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Development of a Model to Predict Chemical Permeation of the U.S. Coast Guard Chemical Response Suit

R. Goydan and J.R. Powell

Arthur D. Little, Inc.
15 Acorn Park
Cambridge, MA 02140-2390

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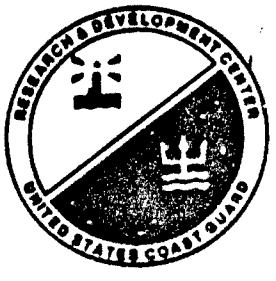

SAMUEL F. POWEL, III
Technical Director
United States Coast Guard
Research & Development Center
1082 Shennecossett Road
Groton, CT 06340-6096

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16. Abstract

A predictive model was developed and computerized to enable Coast Guard field personnel to determine with 95% certainty whether totally encapsulated suits would be adequate barriers to untested chemicals. The model was based on permeation test results at 25 degrees centigrade of 163 chemicals against Challenge 5100 and 125 chemicals against Challenge 5200 fluoropolymer suit materials. Additional tests contained in the data base included tests at other temperatures and 36 mixtures.

The model enables prediction as to whether permeation will be detected within three hours at 25 degrees centigrade, based on structure and size of the chemical of interest. Mixtures were found to exhibit no synergistic effects, i.e., each component behaves as it would alone (permeates or does not permeate). Compounds that tend to permeate have six carbons or less, carbon-carbon multiple bonds, halogen atoms, and are small non-polar organic compounds or small non-acidic, non-ionic inorganic compounds.

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METRIC CONVERSION FACTORS

Approximate Conversions to Metric Measures

Symbol	When You Know	Multiply By	To Find	Symbol
		LENGTH		
in	inches	* 2.5	centimeters	cm
ft	feet	30	centimeters	cm
yd	yards	0.9	meters	m
mi	miles	1.6	kilometers	km
		AREA		
in^2	square inches	6.5	square centimeters	cm^2
ft^2	square feet	0.09	square meters	m^2
yd^2	square yards	0.8	square meters	m^2
mi^2	square miles	2.6	square kilometers	km^2
	acres	0.4	hectares	ha
		MASS (WEIGHT)		
oz	ounces	28	grams	g
lb	pounds	0.45	kilograms	kg
	short tons (2000 lb)	0.9	tonnes	t
		VOLUME		
tsp	teaspoons	5	milliliters	ml
tbsp	tablespoons	15	milliliters	ml
fl oz	fluid ounces	30	milliliters	ml
c	cups	0.24	liters	l
pt	pints	0.47	liters	l
qt	quarts	0.95	liters	l
gal	gallons	3.8	liters	l
ft^3	cubic feet	0.03	cubic meters	m^3
yd^3	cubic yards	0.76	cubic meters	m^3
		TEMPERATURE (EXACT)		
°F	Fahrenheit temperature	5/9 (after subtracting 32)	Celsius temperature	°C

*1 in = 2.54 (exactly). For other exact conversions and more detailed tables, see NBS Misc. Publ. 286, Units of Weights and Measures. Price $2.25.
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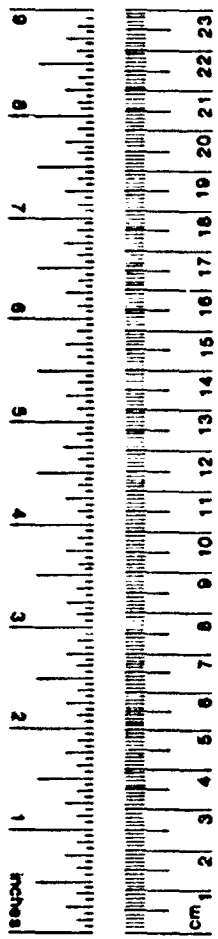
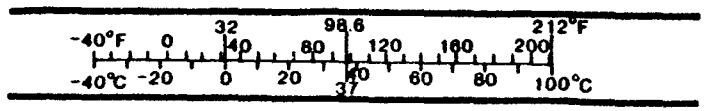


Approximate Conversions from Metric Measures

Symbol	When You Know	Multiply By	To Find	Symbol
		LENGTH		
mm	millimeters	0.04	inches	in
cm	centimeters	0.4	inches	in
m	meters	3.3	feet	ft
m	meters	1.1	yards	yd
km	kilometers	0.6	miles	mi
		AREA		
cm^2	square centimeters	0.16	square inches	in^2
m^2	square meters	1.2	square yards	yd^2
km^2	square kilometers	0.4	square miles	mi^2
ha	hectares (10,000 m^2)	2.5	acres	
		MASS (WEIGHT)		
g	grams	0.035	ounces	oz
kg	kilograms	2.2	pounds	lb
t	tonnes (1000 kg)	1.1	short tons	
		VOLUME		
ml	milliliters	0.03	fluid ounces	fl oz
l	liters	0.125	cups	c
l	liters	2.1	pints	pt
l	liters	1.06	quarts	qt
l	liters	0.26	gallons	gal
m^3	cubic meters	35	cubic feet	ft^3
m^3	cubic meters	1.3	cubic yards	yd^3
		TEMPERATURE (EXACT)		
°C	Celsius temperature	9/5 (then add 32)	Fahrenheit temperature	°F



CONTENTS

TABLES

TABLES
(continued)

FIGURES

SECTION 1

EXECUTIVE SUMMARY

1.1 INTRODUCTION

Emergency spill response personnel wear protective clothing to minimize exposures to potentially hazardous chemicals. Consequently, the materials used to construct the clothing must provide superior chemical resistance, preferably to the broad range of chemicals that are used in commerce. One high performance encapsulating suit is the U.S. Coast Guard's Chemical Response Suit (CRS) in which the principal material of construction is a fabric with fluoropolymer films on its surfaces (Challenge® 5100 and Challenge® 5200, Chemical Fabrics Corporation). Permeation testing has demonstrated that these fabrics provide good resistance to a wide range of chemicals, however, some chemicals do permeate the fabrics. Since there is virtually an unlimited number of chemicals and chemical mixtures and because testing of all such potential challenges is impractical, there was the desire to develop a predictive model to provide reasonable estimates of the permeation resistance. The development of such a model could lead to targeted decisions as to which chemicals and mixtures should be tested, better clothing selection decisions, and improved worker safety.

1.2 PERMEATION DATA FASE

The results of over 300 tests were provided by the Coast Guard on the permeation of a broad range of pure chemicals and chemical mixtures through Challenge 5100 and 5200. Although the Challenge materials contain different substrates (aramid vs. glass fiber), the outer, fluoropolymer film layers appear to be the same total thickness, approximately 0.008 cm, as measured by cross-section.

The permeation tests had been performed in accordance with ASTM Method F739-85. Early tests were continued until steady-state permeation rates were achieved, however, the majority of the tests was terminated at 3 hours. The 3-hour limit was specified because it is the maximum duration for Coast Guard CRS use. Breakthrough times and permeation rates as a function of time were measured. However, permeation versus time curves or raw data were not made available to us for all material/chemical combinations tested. In general, the method detection sensitivity was less than 0.05 $\mu g/cm^2$-min but did vary for each chemical and sometimes varied in subsequent tests with the same chemical. The lack of a constant detection sensitivity and single test duration made it difficult to develop a model to quantitatively predict the permeation behavior, particularly regarding breakthrough times. Definition of a standard breakthrough detection sensitivity for permeation testing is now under consideration by the ASTM and, if adopted, would facilitate the comparison of permeation test results.

At 25°C, permeation test results were reported for 163 chemicals for Challenge 5100 and 125 chemicals for Challenge 5200. Permeation test results were also reported for a small number of tests at 30°, 35°, and 40°C. The Coast Guard data set also included results for

permeation tests conducted with 29 chemical mixtures, however, only breakthrough times were measured. To further expand the mixture permeation data base, supplementary mixture tests were conducted by Arthur D. Little. Permeation tests were conducted for five, two-component and two, three-component mixtures. In these tests, the permeation rate of each mixture component was measured as a function of time.

1.3 PURE CHEMICAL PERMEATION

For Challenge 5100, permeation was detected within 3 hours for 20 of the 163 chemicals. For Challenge 5200, permeation was detected for 47 of the 128 chemicals. In general, permeation results for chemicals tested against both materials were similar although Challenge 5100 may provide a slightly better barrier. Thus, in our analysis and model development efforts, we treated the materials as equivalent and combined the data sets. Permeation rate versus time curves were available to us for most of the tests in which permeation was detected. We first analyzed the curves to assess the permeation mechanism.

1.3.1 Permeation Mechanism

The permeation-time curves were analyzed to determine whether the permeation was controlled by a solution-diffusion process or was occurring by some other mechanism. Mathematical relationships based on Fick's law were used to calculate values for the solubility (S) and the diffusion coefficient (D) from the permeation-time data. For the 35 cases studied, an excellent fit to the permeation data was possible using Fick's law with a constant D. For these chemicals, the D values ranged from 10^{-10} to 10^{-9} cm^2/s and the S values generally ranged from 0.0001 to 1.0 g/cm^3. On this basis, we concluded that the permeation process was occurring by a solution-diffusion mechanism. The small set of permeation curves for analysis, and the lack of well-developed methods for predicting D and S for chemicals in fluoropolymers at present, limited the development of a quantitative model for predicting permeation behavior. Consequently, our focus was to develop an empirical model to predict the permeation behavior. We also analyzed the permeation-time curves for the chemicals tested at multiple temperatures to investigate the effect of temperature. The data set, however, was inconsistent and no quantitative conclusions could be reached regarding the effect of elevated temperature on the permeation resistance.

1.3.2 Predictive Model

Using the full permeation database measured at 25°C, we developed an empirical model to predict permeation of Challenge 5100 or Challenge 5200 within 3 hours at 25°C at a representative detection sensitivity of 0.05 $\mu g/cm^2$-min. We explored correlations with the chemical's structure, size, and shape. We found that the simplest and most accurate model was one based on chemical structure that addresses both molecular size and electronic structure. In general, chemicals with 6 or greater non-hydrogen atoms do not permeate the Challenge materials. Compounds of small size and with the following structure types tend to permeate:

- carbon-carbon multiple bonds (non-aromatic),
- halogen atoms (F and Cl),
- small non-acidic, non-ionic inorganic compounds, or
- small non-polar organics.

Thus, a set of rules was developed, in the form of questions with yes or no answers regarding chemical structure that leads to a Yes/No prediction of permeation. The set of rules was applied to the present data base and was found to accurately predict the behavior for 88% to 93% of the chemicals tested. The rules were organized into a decision tree and programmed for use on a personal computer.

1.4 CHEMICAL MIXTURE PERMEATION

The permeation data for 29 chemical mixtures provided by the Coast Guard included both two- and three-component mixtures. The behavior can be summarized as follows. If a mixture component was found to permeate when tested as a pure chemical, it was found to permeate from the mixture and at approximately the same or slightly longer breakthrough time. If the mixture component did not permeate when tested as a pure chemical, it also was not found to permeate from a mixture. No synergistic effects were observed.

To better understand mixture permeation, we conducted supplementary tests that involved two- and three-component mixtures of three chemicals to explore the effect of concentration on the mixture permeation behavior. The permeation rates as a function of time of the mixture components were generally proportional to their concentration in the mixture (i.e., as the concentration was decreased, the breakthrough time increased and the steady-state permeation rate decreased).

1.4.1 Predictive Model

Although based on a limited data set, a general rule was developed to predict chemical mixture permeation through the Challenge materials, again at 25°C and within 3 hours, as follows. If the chemical permeates in pure form, it will permeate from a mixture at a permeation rate proportional to its concentration in the mixture. If the chemical does not permeate in pure form, it will not permeate from a mixture.

1.5 COMPUTERIZED PREDICTION MODEL AND DATABASE

A computerized version of the permeation data set and prediction model was developed using SuperCard 1.5 (Silicon Beach Software) to run on Macintosh computers. For every chemical entered into the database, there is one card that stores information on the chemical identity, permeation data (if available), and permeation model prediction (if generated.) System operational features include capabilities to search the database, run the permeation prediction model, enter data or model predictions into the database (access to this feature is restricted), and print entries from the database. A user manual was also developed.

1.6 CONCLUSIONS AND RECOMMENDATIONS

The permeation resistance of Challenge 5100 and Challenge 5200 has been widely tested and the results indicate that these materials are effective barriers to a broad range of chemicals and chemical mixtures. When permeation was detected, it was found to follow a simple Fickian diffusion mechanism with a constant diffusion coefficient. No quantitative predictive model based on the Fick's law approach was developed however. Also, no definitive conclusions could be reached regarding the effect of temperature on the permeation resistance of the Challenge materials based on the available data set.

An empirical model or rule system was developed that enables the prediction as to whether permeation will be detected within three hours at 25°C based on the structure and size of the chemical of interest. Based on a smaller set of data, the permeation of mixtures or the components thereof was found to behave similarly to the results for the chemicals tested individually. If a chemical permeates the Challenge material as a pure chemical then it will permeate from a mixture. Conversely, if a chemical does not permeate in pure form then it will not permeate from a mixture.

A computerized version of the permeation database and prediction model was developed for use by personnel with minimal permeation or chemistry training. The computer system should facilitate thorough and efficient reviews of existing data and assessments of probable permeation behavior by field (or other) users who must make clothing selection decisions. Although use of the model was targeted as an aid for making clothing selection decisions, it is also useful to focus decisions regarding priority chemicals and mixtures for future testing.

Further research should be undertaken to address some of the uncertainties in the data set, the predictive model described herein, and other approaches being evaluated to predict the permeation behavior. Specific recommendations include:

- A field evaluation of the computerized permeation database and predictive model should be undertaken to assess the product's usefulness and identify ways to optimize the product to better meet Coast Guard's needs.

- Future permeation tests, if performed, should be conducted so that chemical breakthrough is determined at a constant, normalized permeation detection rate, if feasible.

- Selected permeation tests at elevated temperatures should be repeated to confirm the results reported to date and to better understand the effect of temperature on the permeation resistance of the Challenge materials.

- Permeation tests with additional chemical mixtures should be undertaken to further validate the mixture permeation rule.

- The computerized permeation database should be updated as more data are generated and the predictive model should be continually tested as new data become available to expand and improve its accuracy.

- In the long term, similar computer databases and predictive models could be developed for other important components of the Coast Guard CRS (e.g., glove materials, face shield material) or alternative materials for the encapsulating suit fabric that may adopted at a later date. Development of such databases and models provide a better understanding of the barrier properties of critical materials and help to focus priorities for testing.

SECTION 2

INTRODUCTION

2.0 BACKGROUND

Since 1978, the U.S. Coast Guard has been responsible for inspecting marine chemical-transporting vessels and responding to chemical spills into waters in the United States. At that time, a research and development project was initiated to develop chemical protective clothing and equipment for use during spill response activities. Because of the variety of chemicals that are handled in commerce, the Coast Guard required a protective clothing ensemble that was an effective barrier to a broad range of chemicals. For example, the Coast Guard's Chemical Hazard Response Information System (CHRIS) includes spill response information for over 1100 chemicals [1]. Early, commercially-available protective ensembles and materials that were evaluated included butyl rubber, Viton/chlorobutyl laminate, and chlorinated polyethylene [2,3]. In general, these materials were found to provide only fair resistance to the CHRIS chemicals.

In the mid-1980s, the Coast Guard renewed its search for improved protective materials and identified a proprietary fluoropolymer-film based composite fabric, Challenge 5100. To support the development of an ensemble using this material, an extensive testing program was undertaken to assess the fabric's performance as a primary suit material [4]. In addition to chemical resistance evaluations, the program involved evaluation of physical properties, critical suit seams, other suit components, etc., that will not be considered here.

To evaluate the chemical resistance of the Challenge 5100 material, a permeation test program was undertaken by the Coast Guard Research and Development Center beginning in 1985 and continuing through 1990 [5,6]. During that time, a second fabric, the Challenge 5200 material, was introduced and incorporated into the testing program. In general, good resistance to permeation was demonstrated in over 300 permeation tests with these fabrics for a wide range of chemicals. Since there is virtually an unlimited number of chemicals and chemical mixtures and because testing of all potential challenges is impractical, there was the desire to develop a predictive model to provide reasonable estimates of the permeation resistance.

2.1 OBJECTIVE

The objective of this project was to develop a model to predict permeation of the Challenge materials based on the permeation data set available from the Coast Guard. At the minimum, the model was to predict whether measurable permeation will or will not occur after a specified duration. If sufficient data were available and the permeation process occurred by a solution-diffusion process, a further objective was to develop a model that accurately predicts permeation behavior as a function of time.

2.2 SCOPE AND APPROACH

The permeation model developed in this study is based on permeation data provided by the Coast Guard as well as a small set of chemical mixture permeation data generated in our laboratories. Our approach was to compile and analyze the permeation data set, assess the permeation mechanism, and then develop, test, and refine a predictive model. Much of our initial effort was directed toward compiling and analyzing the data set, which was reported in a series of reports and using a series of formats. Also, additional data were being reported to us throughout the model development program.

Both theoretical and empirical approaches to a predictive model were investigated. Initially the emphasis was on theoretical approaches based on Fick's laws of diffusion since, if successful, such models can be extrapolated with greater confidence to conditions other than those considered in the model development. In addition, we investigated empirical approaches including correlations with chemical structure, size, and shape. The ultimate goal was a generalized model that could be applied rapidly and reliably by field personnel who must make clothing selection decisions. In addition to developing a model to predict pure chemical permeation, we also analyzed two smaller data sets, one for mixtures and one for tests at elevated temperature, to investigate the effects of temperature and mixture composition on the permeation behavior.

The program began with a model development phase based on a review of the existing data set. At the conclusion of this phase, a prototype model was proposed and a series of chemical permeation tests were recommended to test the prototype model. The results of these tests were then used to refine the prototype model and establish the accuracy and limitations of the final model. At the conclusion of the effort, a computerized version of the data set and the predictive model were developed to facilitate its use in the field.

SECTION 3

PERMEATION DATA SET

3.1 CRS MATERIALS TESTED

Since 1985, the Coast Guard has been evaluating the suitability of two proprietary fabrics to meet their requirements for a totally encapsulating suit material. The two materials are manufactured by the Chemical Fabrics Corporation (Merrimack, NH) and involve composite structures in which outer, fluoropolymer (Teflon®) films provide the chemical resistance. Challenge 5100, the first of these materials, is a composite structure of fluoropolymer films applied to both sides of a woven aramid reinforcing substrate. The second material, Challenge 5200, is a similar composite structure with the outer, fluoropolymer films applied to a glass fiber reinforcing substrate.

Preliminary evaluation of the Challenge 5100 material indicated very good resistance to chemical permeation and good physical properties relative to those of other materials that the Coast Guard had previously evaluated [4]. Consequently, the Challenge 5100 material was selected for an extensive testing program, one aspect of which was to evaluate the permeation resistance of the material to a large set of priority chemicals [5,6]. In the midst of this testing program the manufacturer introduced the Challenge 5200 material, as a next generation version of the Challenge 5100 material, and this new material was incorporated into the Coast Guard testing program [7].

Although requested, the manufacturer would not provide information regarding the fluoropolymer composition, barrier layer thicknesses, or whether differences exist between the fluoropolymer films of the fabrics. Rough measurements were made in our laboratory to compare the barrier layer thicknesses, however, no analyses were undertaken to compare the fluoropolymer layer compositions. Fluoropolymer layer thicknesses were estimated by examination of the materials' cross-section using a microscope:

- Challenge 5100
  - total composite thickness: 0.048 cm
  - outer fluoropolymer layer: 0.0045 cm
  - inner fluoropolymer layer: 0.0035 cm
  - total fluoropolymer thickness: 0.0080 cm

- Challenge 5200
  - total composite thickness: 0.026 cm
  - outer fluoropolymer layer: 0.0040 cm
  - inner fluoropolymer layer: 0.0040 cm
  - total fluoropolymer thickness: 0.0080 cm

The presence of fluoropolymer layers on both the inner and outer surfaces of the materials was confirmed by attenuated total reflectance (ATR) infrared analysis of the sample surfaces.

Based on these measurements, the two fabrics appear to contain the same total fluoropolymer film thickness even though Challenge 5200 is approximately one half the thickness of Challenge 5100. As discussed later, comparison of the permeation test results for the two materials appear to support this conclusion.

3.2 PERMEATION TEST METHOD AND DATA REPORTING FORMAT

The majority of the permeation test data analyzed in this effort was generated by Texas Research International (TRI) under contract to the Coast Guard [6,7]. Essentially all tests with pure chemicals, several tests at elevated temperatures and most of the chemical mixture tests were performed by TRI. Some early tests were conducted by the Coast Guard Research and Development Center. A small number of mixture permeation tests were performed by Arthur D. Little and are described in Section 3.2.2. In general, the permeation tests were conducted in accordance with ASTM F739-85 but with minor modifications in some cases.

3.2.1 Tests Performed by Texas Research International

Most tests conducted by TRI were performed using an automated permeation test system in which three test replicates were performed simultaneously. The system uses an open-loop testing mode with photoionization detection. In general, the collection medium flow rate was set at 100 cc/min. In most tests, a 2.54 cm diameter test cell was used, however, in many of the early tests the ASTM F739 standard cell of 5.08 cm diameter was used. The small diameter cell has a 5.07 cm^2 exposed surface area whereas the 5.08 cm diameter cell has a 20.3 cm^2 area. Alternative detection methods were used for chemicals that could not be detected by photoionization.

After charging the challenge side of the permeation cell with the test chemical, the collection side of the test cell was monitored periodically. In early tests (i.e., most of the Challenge 5100 tests), the detector responses were monitored for 3 hours or until a steady-state permeation rate was achieved in tests in which permeation was detected within 3 hours. In later tests (i.e., most of the Challenge 5200 tests), the detector responses were monitored for 3 hours (although sometimes this was extended to 4 to 7 hours). For tests in which permeation was detected but steady-state was not reached within 3 hours, the maximum permeation rate measured during the test was reported. As discussed later, there were very few cases in which the permeation rate reached steady-state within 3 hours.

The results of the permeation tests were reported to us by the Coast Guard in various summary reports, summary tables, and individual data sheets with attached instrument response curves over the course of this program. A significant portion of our efforts involved compiling the reported results into a consistent format and analyzing the data set to understand the permeation behavior.

Breakthrough was determined to occur by TRI when the detector response exceeded a minimum detectable limit (MDL). The detector response was calibrated separately for each chemical using a syringe pump and single point calibration technique [8]. The detector

response (mV) was used to calculate the response factor (mV/ppm) and the MDL in concentration units of parts per million (ppm). The response factor, determined at a single low concentration, was assumed to be a linear response with a zero intercept and used as a constant to convert the detector responses measured in the permeation test to concentration values. The concentration values were converted to permeation rates using the collection medium flowrate and the clothing material surface area. In most cases, only the final permeation rate was reported in permeation rate units. The results as a function of time were reported in graphs showing detector response (mV) plotted versus time. From these curves, we converted the response data to permeation rates as a function of time for our analyses. Because response factors (mV/ppm) were not reported to us for all chemicals, we converted the instrument response graphs using the reported permeation rate value and the mV response reading at that time. Thus, there may be some uncertainty in our values as a function of time.

Several tests with chemical mixtures were also performed. These tests involved binary and ternary mixtures of liquid chemicals and were conducted using the automated system described above. In these tests, only breakthrough times were reported. In several tests, however, only a generic MDL and breakthrough time were reported without identifying which component had actually broken through. No permeation rate or instrument response data as a function of time were provided to us for these tests.

In summarizing the data set, it is important to note that an individual MDL value was determined for each chemical/test and used to judge whether permeation occurred. MDL values ranged from 0.001 ppm to 40 ppm depending upon the instrument sensitivity for the chemical of interest. In several cases in which tests were repeated for the same chemical (or performed with both Challenge 5100 and 5200), the reported MDLs for that chemical varied by several orders of magnitude. This range makes it difficult to compare the results of tests in which permeation was not detected. To better normalize the data set, we converted the MDL values from concentrations (ppm) to minimum detectable permeation rate (MDR) values in units of $\mu g/cm^2$-min using the reported flowrates and exposed surface areas. Use of MDRs eliminates some apparent discrepancies in the data set and allows for more direct comparison of the results [9]. In particular, this was important when comparing results in which permeation was or was not detected at apparently the same MDL but at different test conditions. As discussed later, this data set illustrates the difficulty in interpreting permeation test results when a constant detection limit (i.e., MDR) is not used and many tests are terminated before permeation is detected. Consequently, throughout this report, the data tables reporting breakthrough times and permeation rates, also report the detection limit for the chemical and the duration of the permeation test.

3.2.2 Tests Performed by Arthur D. Little

To further expand the chemical mixture database, supplementary permeation tests were conducted by Arthur D. Little under this contract. Permeation tests were conducted for seven different mixtures involving carbon disulfide, vinyl acetate, and ethanol. The standard ASTM F739 permeation test cell was used providing a clothing material surface area of 20.3 cm^2. The tests were conducted in a closed-loop mode with air as the collection medium. The total

collection medium volume was 6 liters and was continuously recirculated at a rate of 10 liters/min for the test duration. A Miran 80A Infrared Spectrophotometer (Foxboro Company, Foxborough, MA) was employed to detect the concentration of the chemical in the collection medium. Calibration curves of concentration (μg/L) versus absorbance were generated over the range of expected concentration values. Individual MDLs and MDRs were determined for the three test chemicals. The spectrophotometer was calibrated prior to testing each day that tests were conducted.

All tests were performed until either each component of the mixture being tested reached a steady-state permeation rate or eight hours had elapsed. Only ethanol failed to reach steady-state in this time period. In all cases, the permeation rates as a function of time were recorded so that the effect of mixture composition and concentration on the permeation behavior could be observed.

3.3 PURE CHEMICAL DATA SET

3.3.1 Summary

The results of permeation tests conducted with over 300 chemical/material combinations were available for analysis in this study. As noted earlier, the results of the permeation tests were reported to us by the Coast Guard in various summary reports, summary tables, and individual data sheets during this program. Thus, the compilation and analysis of the test results continued throughout the model development effort.

Table 1 summarizes the permeation tests that were conducted at (or near) 25°C. In total, 163 chemicals were tested against Challenge 5100 while only 128 chemicals were tested against Challenge 5200. Of these, only 39 chemicals were tested against both materials. Complete tables of the permeation test results, as compiled by us, are provided in Appendix A with Table A-1 reporting the Challenge 5100 results and Table A-2 reporting the Challenge 5200 results. Table A-2 also includes results for 21 chemicals that were reported by the manufacturer, Chemical Fabrics Corporation [10]. Most of these chemicals were also tested by TRI. The source of the data is indicated in the Appendix A tables. Permeation tests were also conducted at elevated temperatures with Challenge 5200 as summarized in Table 2. These tests were conducted at 30°, 35°, and 40°C using chemicals that, in general, had also been tested at 25°C. Complete tables of the permeation test results, again as compiled by us, are provided in Appendix B.

The Appendix A and Appendix B tables report the chemical name, the MDL (ppm), the MDR (μg/cm^2-min), and the permeation test results in terms of the average breakthrough time (min) average reported permeation rate (μg/cm^2-min), an indicator as to whether the rate was at steady-state or at the test conclusion, and the breakthrough times and permeation rates reported for each of the three replicate tests, when applicable. In approximately 20% of the cases, permeation-time curves were not provided so we could not conclude whether permeation had reached steady-state. These cases are noted in the tables. In general, the permeation-time curves that were received showed instrument responses that increased smoothly from the baseline over time. Several curves, however, showed a lot of noise,

TABLE 1. SUMMARY OF PERMEATION TESTS AT 25°C

Condition	No. of chemicals	
	Challenge 5100	Challenge 5200
Total chemicals tested	163	128
- Chemicals tested multiple times	11	22
Chemicals for which permeation was detected within 3 hours	20	47
- Chemicals for which curves for permeation as a function of time were provided	18	37
- Chemicals for which permeation rate reached steady-state	10	6
- Chemicals for which the test was terminated before steady-state*	8	31

* Typically 3-hour test duration.

TABLE 2. SUMMARY OF PERMEATION TESTS FOR CHALLENGE 5200 AT ELEVATED TEMPERATURES

Condition	No. of chemicals		
	30°C	35°C	40°C
Total chemicals tested	18	20	9
- Chemicals tested multiple times	1	0	0
Chemicals for which permeation was detected within 3 hours	8	10	7
- Chemicals for which curves for permeation as a function of time were provided	0	9	7
- Chemicals for which permeation rate reached steady-state	**	0	1
- Chemicals for which the test was terminated before steady-state*	**	9	6

* Typically 3-hour test.
** Unknown because permeation-time curves were not provided.

spikes, or drifting behavior and were considered unusable results. These tests were discussed with the Coast Guard and, in several cases, repeated.

The numbers of chemicals that were tested multiple times are noted in Tables 1 and 2. The results of these repeat tests are compared in Table 3 for Challenge 5100 and in Table 4 for Challenge 5200. In general, the reproducibility was only fair and was better for Challenge 5100. For the 11 chemicals tested multiple times with Challenge 5100, seven were either in good agreement or the lack of agreement could be related to differences in the detection limit (or possibly the test temperature, 25° vs. 27°C). For example, in the first test with acetone, no permeation was detected at 25°C within 210 minutes at an MDR of 0.047 $\mu g/cm^2$-min. In the repeat test, permeation was detected at 27°C at an average of 71 minutes at an MDR of 0.00004 $\mu g/cm^2$-min, an MDR that is three orders of magnitude lower. In other cases, discrepancies exist within replicates or reported permeation rates varied by several orders of magnitude. For the 22 chemicals tested multiple times against Challenge 5200, the results for about ten were in good agreement or their differences could be related to MDR differences. But, as Table 4 illustrates, there are also over ten cases in which either the repeat results do not agree regarding breakthrough time or the reported permeation rate values differ by over an order of magnitude. The testing laboratory suggests that the variations are due to differences in the lots of the Challenge materials tested.

This lack of reproducibility in some of the data set confounded our analyses and limited attempts to develop a model to predict quantitative breakthrough times or permeation rates. Thus, as detailed in Section 4, our model development efforts ultimately focussed on developing an empirical model that predicts whether permeation will be detected at a representative MDR within 3 hours at 25°C. Only a small effort was undertaken to predict the permeation behavior as a function of time for the chemicals found to permeate.

3.3.2 Chemicals for Which Permeation Was Detected at 25°C

For Challenge 5100, 20 chemicals were found to permeate within 3 hours, at their reported MDRs. The test results for these chemicals are summarized in Table 5. For ten of these chemicals, the permeation-time curves show that permeation had reached steady-state, often at much longer than 3 hours. In comparison, 47 of the 128 chemicals tested against Challenge 5200 were detected to permeate within 3 hours. The test results for these chemicals are reported in Table 6. For this fabric, only 6 tests were continued until steady-state. The remaining permeation tests were terminated at 3 hours (or longer in some cases.)

The larger percentage of chemicals that permeate Challenge 5200 material is not necessarily because Challenge 5200 is a less resistant barrier but could be because the chemicals tested against Challenge 5200 were more carefully selected, from a permeation standpoint, based on earlier Challenge 5100 test results. Most of the Challenge 5100 results had been obtained before the start of this program whereas the Challenge 5200 testing continued throughout the model development effort. Thus, as the Coast Guard began to understand better the permeation behavior of Challenge 5100, it began to specify testing with chemicals that had a higher probability of permeating Challenge 5200 [20]. In Tables 5 and 6, the chemicals tested after our preliminary model was developed are indicated with a (+).

TABLE 3. SUMMARY OF REPEAT PERMEATION TESTS WITH CHALLENGE 5100 AT 25°C

Chemical name	Test #	MDL* (ppm)	MDR* ($\mu g/cm^2$-min)	Average BT (min)	Average reported rate** ($\mu g/cm^2$-min)	
Acetone	1	1.2	0.047	>210	--	
(27°C)	2	0.001	0.00004	71	1.6	(3hr)
Acetonitrile	1	nd	nd	>270	--	
	2	1.0	0.033	>180	--	
Allyl Chloride	1	0.16	0.0025	134	0.011	(ss)
	2	0.060	0.0037	143	0.013	(6hr)
Ammonium Hydroxide	1	2.0	0.057	30, >180†	26.7	(3hr)
	2	7.2	0.020	>180	--	
1,2-Dichloroethylene	1	0.010	0.0008	15	1.1	(ss)
	2	0.010	0.0008	23	0.13	(ss)
Dichloromethane	1	0.27	0.0042	51	0.020	(ss)
(USCG)	-	0.030	*	61	nd	
Ethyl Ether	1	0.13	0.0078	>180	--	
	2	0.010	0.0006	92	0.005	(3hr)
(27°C)	3	0.006	0.0004	117	1.07	(3hr)
Sodium Hydroxide, 50%	1	0.50	0.016	>180	--	
(USCG)	-	nd	nd	>4260	--	
Tetrachloroethylene	1	0.11	0.015	>624	--	
(USCG)	-	nd	nd	108	nd	
(27°C)	2	0.001	0.0001	26, >180†	18.0	(3hr)
Trichloroethylene	1	0.070	0.0017	148	0.031	(ss)
	2	0.010	0.0011	138	0.031	(6hr)
Vinylidene Chloride	1	0.49	0.038	>180		
	2	0.010	0.0008	51	0.022	(3hr)

* MDL = minimum detectable concentration determined by syringe pump calibration; MDR = minimum detectable permeation rate calculated from MDL, carrier gas flowrate, and material surface area. Values entered as (*) could not be converted, (nd) indicates not determined.

** Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value.

† Conflicting results were measured within the three replicates for this test.

TABLE 4. SUMMARY OF REPEAT PERMEATION TESTS WITH CHALLENGE 5200 AT 25°C

Chemical name	Test #	MDL* (ppm)	MDR* (µg/cm²-min)	Average BT (min)	Average reported rate** (µg/cm²-min)	
Acetone	1	1.0	0.040	>180	--	
(27°C)	2	0.010	0.0004	116	0.0004	(3hr)
(27°C)	3	0.001	0.00004	>180	--	
(ChemFab)	-	0.10	*	>300	--	
Ammonia Gas	1	0.30	0.0041	31	0.11	(ss)
	2	0.070	µL 0.0010	25	0.24	(3hr)
(27°)	3	0.030	µL 0.0004	32	0.15	(3hr)
(ChemFab)	-	0.10	*	>300	--	
Ammonium Hydroxide	1	0.25	0.0071	>180	--	
(27°C)	2	7.2	0.20	120	0.34	(3hr)
Benzonitrile	1	0.010	0.0008	>180	--	
	2	0.020	0.0017	>180	--	
1,3-Butadiene Gas	1	0.068	0.0030	5	0.039	(5hr)
	2	0.010	µL 0.00044	24	0.080	(3hr)
Chlorine Gas	1	1.0	0.057	70	0.020	(nc)
	2	38.0	2.2	60	170.3	(nc)
(ChemFab)	-	0.30	*	>300	--	
Cyclopropane Gas	1	0.020	µL 0.0007	92	0.0008	(3hr)
(27°C)	2	0.002	0.0001	78	0.0008	(3hr)
Dichloromethane	1	0.005	0.0003	64	0.26	(3hr)
(27°C)	2	0.007	0.0005	83	3.7	(3hr)
(ChemFab)	-	0.10	*	64	0.12	
Dimethyl Sulfide	1	0.010	0.0008	95	0.0005	(3hr)
	2	0.010	0.0008	48	0.0002	(3hr)
Ethanethiol	1	0.020	0.0010	65	0.0028	(3hr)
(27°C)	2	0.003	0.0002	83	15.3	(3hr)
Ethyl Ether (27°C)	1	0.010	0.0006	127	0.38	(20hr)
(27°C)	2	0.010	0.0006	92	0.0080	(3hr)
(27°C)	3	0.003	0.0002	149	2.1	(3hr)
(27°C)	4	0.010	0.0006	40	173.3	(3hr)
Ethylene Oxide Gas	1	3.0	0.11	57	0.73	(3hr)
	2	0.65	0.023	25	0.14	(3hr)
(ChemFab)	-	0.34	*	64	0.76	

(continued)

TABLE 4. SUMMARY OF REPEAT PERMEATION TESTS WITH CHALLENGE 5200 AT 25°C

Chemical name	Test #	MDL* (ppm)	MDR* (µg/cm²-min)	Average BT (min)	Average reported rate** (µg/cm²-min)	
Hydrogen Sulfide Gas	1	0.030	0.0008	4	0.0028	(3hr)
(27°)	2	0.010	0.0003	8	0.0070	(3hr)
	3	0.030	0.0008	15	0.0078	(nc)
Methyl Bromide Gas	1	0.40	0.031	21	0.035	(3hr)
	2	0.020	µL 0.0015	20	0.0065	(3hr)
Methyl Chloroformate	1	0.050	0.0038	81	0.012	(3hr)
(27°C)	2	0.10	0.0076	95	0.95	(3hr)
Nitromethane	1	0.73	0.036	168	0.054	(nc)
	2	0.70	0.035	>180	--	
Sulfur Dioxide Gas	1	47.0	mL 0.020	60	0.090	(3hr)
	2	1.0	mL 0.052	40	2.3	(3hr)
Trichloroethylene	1	0.010	0.0011	49	0.19	(3hr)
(27°C)	2	0.010	0.0011	72	0.0028	(3hr)
Trimethylamine	1	0.15	0.0072	20	nd	(nc)
	2	0.014	0.0007	>180	--	
	3	0.15	0.0072	25	nd	(nc)
Vinyl Acetate	1	0.020	0.0014	69	0.25	(nc)
	2	0.004	0.0003	73	38.0	(3hr)
	3	0.004	0.0003	109	11.3	(3hr)
Vinyl Chloride Gas	1	0.010	µL 0.0005	12	0.084	(3hr)
	2	0.020	µL 0.0010	7	0.060	(3hr)
Vinylidene Chloride	1	0.49	0.038	124	1.1	(3hr)
(27°C)	2	0.010	0.0008	40	0.086	(3hr)
	3	0.030	0.0023	61	0.082	(3hr)

* MDL = minimum detectable concentration determined by syringe pump calibration; MDR = minimum detectable permeation rate calculated from MDL, carrier gas flowrate, and material surface area. Values entered as (*) could not be converted, µL indicates values reported as µL instead of µg, (mL) indicates mL instead of µg.

** Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value, and (nc) indicates that no permeation time curve was provided.

TABLE 5. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5100 AT 25C

Chemical+	MDL* (ppm)	MDR* (µg/cm²-min)	Average BT (min)	Average Reported rate** (µg/cm²-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (µg/cm²-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (µg/cm²-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (µg/cm²-min)
Acetone	1.160	0.0469	> 210							
Acetone (27C) +	0.001	0.00004	71	1.630 (3hr)	44	1.3000	104	1.2000	64	2.4000
Acrolein	0.120	0.0054	41	0.033 (ss)	44	0.0395	38	0.0268		
Acrylonitrile	0.460	0.0049	65	0.014 (ss)	54		76	0.0143		
Allyl Chloride	0.160	0.0025	134	0.011 (ss)	102	0.0107	166	0.0103		
Allyl Chloride	0.060	0.0037	143	0.013 (6hr)	136	0.0098	116	0.0210	176	0.0068
Ammonium Hydroxide +	2.000	0.0565	?	(nc)	30	26.6667	> 180		> 180	
Ammonium Hydroxide +	7.200	0.2033	> 180							
Carbon Disulfide	0.100	0.0061	20	0.050 (ss)	22	0.0460	21	0.0608	18	0.0432
Chloroprene (2-Chloro-1,3-Butadiene)	0.030	0.0021	179	0.005 (ss)	192	0.0025	184	0.0032	160	0.0087
1,2-Dichloroethylene	0.010	0.0008	15	1.079 (ss)	20	0.1933	4	2.9333	20	0.1115
1,2-Dichloroethylene	0.010	0.0008	23	0.130 (ss)	21	0.1417	24	0.1177		
Dichloromethane	0.270	0.0042	51	0.020 (ss)	47	0.0228	50	0.0161	55	0.0212
Dichloromethane (USCG R&DC)	0.030	*	61	(nc)	54		65		63	
Ethyl Ether	0.130	0.0078	> 180							
Ethyl Ether +	0.010	0.0006	92	0.005 (3hr)	88	0.0060	84	0.0078	104	0.0012
Ethyl Ether (27C) +	0.006	0.0004	117	1.070 (3hr)	124	1.4000	112	0.9000	116	0.9000
Ethyl Vinyl Ether	0.030	0.0017	113	0.008 (3hr)	148	0.0040	92	0.0117	100	0.0075
Freon 12 (Gas) +	3.500	0.3414 µL	?	(nc)	160	0.0001	> 180		> 180	
Methyl Bromide (Gas) +	0.010	0.0008 µL	27	0.0004 (ss)	28	0.0002	28	0.0005	24	0.0005
Propylene (Gas) +	0.010	0.0003	61	0.0003 (ss)	60	0.0002	48	0.0005	76	0.0002
Propylene Oxide	0.680	0.0080	154	0.021 (ss)	137	0.0238	170	0.0182		
Tetrachloroethylene	0.110	0.0147	> 624							
Tetrachloroethylene (USCG R&DC)	ND	ND	108	(nc)	108					
Tetrachloroethylene (27C) +	0.001	0.0001	?	(3hr)	180		8	33.0000	44	3.0000
Trichloroethylene	0.070	0.0017	148	0.031 (ss)	143	0.0340	156	0.0272	146	0.0318
Trichloroethylene	0.010	0.0011	138	0.031 (6hr)	155	0.0148	140	0.0233	120	0.0540

(Continued)

TABLE 5. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5100 AT 25C

Chemical +	MDL* (ppm)	MDR* (μg/cm²-min)	Average BT (min)	Average Reported rate** (μg/cm²-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (μg/cm²-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (μg/cm²-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (μg/cm²-min)
Vinyl Acetate	0.210	0.0036	106	0.059 (ss)	74	0.0550	137	0.0622		
Vinyl Methyl Ether +	0.540	0.0253	60	2.242 (3hr)	60	3.5833	60	2.3667	60	0.7750
Vinyl-dene Chloride	0.490	0.0383	> 180							
Vinylidene Chloride +	0.010	0.0008	51	0.022 (3hr)	52	0.0117	52	0.0110	48	0.0433

+ Received after initial model development effort.

* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL, the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (*) could not be converted. ND indicates not determined.
Note: μL indicates the MDR and reported rate are in units of μL/cm²-min.

** Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses. (ss) indicates a steady-state permeation rate value. (nc) indicates that no permeation time curve was available.

TABLE 6. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5200 AT 25C

Chemical +	MDL* (ppm)	MDR* (µg/cm²-min)	Average BT (min)	Average Reported rate** (µg/cm²-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (µg/cm²-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (µg/cm²-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (µg/cm²-min)
Acetone	1.000	0.0404	> 180							
Acetone (27C) +	0.010	0.0004	116	0.0004 (3hr)	116	0.0002	116	0.0005	116	0.0005
Acetone (27C) +	0.001	0.00004	> 180							
Allyl Chloride +	0.030	0.0019	56	0.2833 (3hr)	68	0.2867	64	0.1498	36	0.4133
Ammonia (Gas)	0.300	0.0041	31	0.1144 (ss)	36	0.0783	24	0.1583	32	0.1067
Ammonia (Gas) +	0.070	0.0010 µL	25	0.2378 (3hr)	18	0.2683	23	0.2867	35	0.1583
Ammonia (Gas) (27C) +	0.030	0.0004 µL	32	0.1490 (ss)	32	0.1200	32	0.2183	32	0.1100
Ammonium Hydroxide +	0.250	0.0071	> 180							
Ammonium Hydroxide (27C) +	7.200	0.2033	120	0.3390 (3hr)	120	0.2500	120	0.4500	120	0.3167
Bromochloromethane	0.030	0.0031	98	0.0188 (7hr)	93	0.0188	109	0.0147	93	0.0230
Bromoethane	0.010	0.0009	120	0.0281 (3hr)	144	0.0245	84	0.0325	132	0.0272
1,3-Butadiene (Gas)	0.068	0.0030	5	0.0389 (5hr)	8	0.0240	4	0.0375	4	0.0552
1,3 Butadiene (Gas) +	0.010	0.0004 µL	24	0.0795 (3hr)	24	0.1300	24	0.0700	24	0.0383
2-Butene (Gas) (27C) +	0.040	0.0018	55	0.1300 (3hr)	72	0.1000	36	0.2000	56	0.1000
Carbon Disulfide	0.010	0.0006	20	0.0335 (3hr)	20	0.0497	20	0.0208	20	0.0300
Chlorine (Gas) +	1.000	0.0572	70	0.0182 (ss)	90	0.0138	60	0.0267	60	0.0143
Chlorine (Gas) +	38.000	2.1734	60	170.33 (ss)	30	320.00	90	140.00	60	51.0000
Chloroethane +	0.070	0.0036	60	0.6330 (ss)	68	0.3667	52	1.2500	60	0.2833
1-Chloropropane (27C)	2.000	0.1267	260	0.2367 (7hr)	285	0.1433	269	0.2350	225	0.3317
Cyanogen (Gas) +	0.500	0.0210	30	0.0600 (ss)						
Cyclopropane (Gas) +	0.020	0.0007 µL	92	0.0008 (3hr)	96	0.0003	72	0.0013	108	0.0005
Cyclopropane (Gas) (27C) +	0.002	0.0001	78	0.0008 (3hr)	76	0.0008	80	0.0013	80	0.0002
1,2-Dichloroethylene +	0.010	0.0008	24	0.3578 (ss)	28	0.2850	28	0.4050	16	0.3833
cis-1,2-Dichloroethylene	0.010	0.0008	69	0.1550 (3hr)	56	0.2200	80	0.0967	72	0.1483
trans-1,2-Dichloroethylene +	0.010	0.0008	19	1.3967 (ss)	19	1.4317	19	1.4700	19	1.2883
Dichloromethane (27C) +	0.007	0.0005	83	3.6700 (3hr)	84	4.0000	88	3.0000	76	4.0000
Dichloromethane +	0.005	0.0003	64	0.2630 (3hr)	68	0.2300	52	0.3700	72	0.1900
Dimethyl Sulfide +	0.010	0.0008	95	0.0005 (3hr)	116	0.0005	76	0.0005	92	0.0005
Dimethyl Sulfide +	0.010	0.0008	48	0.0002 (3hr)	60	0.0002	40	0.0002	44	0.0003

(Continued)

TABLE 6. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5200 AT 25C

Chemical +	MDL* (ppm)	MDR* (µg/cm²-min)	Average BT (min)	Average Reported rate** (µg/cm²-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (µg/cm²-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (µg/cm²-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (µg/cm²-min)
Ethanethiol +	0.020	0.0010	65	0.0028 (3hr)	60	0.0030	76	0.0025	60	0.0030
Ethanethiol (27C) +	0.003	0.0002	83	15.3300 (3hr)	88	4.0000	88	16.0000	72	26.0000
Ethyl Ether (27C)	0.010	0.0006	127	0.3761 (20hr)	104	0.4050	136	0.3033	140	0.4200
Ethyl Ether (27C) +	0.010	0.0006	92	0.0080 (3hr)	92	0.0143	96	0.0035	88	0.0072
Ethyl Ether (27C) +	0.003	0.0002	149	2.1000 (3hr)	144	4.9000	156	0.9000	148	0.5000
Ethyl Ether (27C) +	0.010	0.0006	40	173.33 (3hr)	44	130.00	36	220.00	40	170.00
Ethyl Vinyl Ether	0.020	0.0012	23	0.6694 (3hr)	40	0.3933	8	0.5517	20	1.0633
Ethylene Oxide (Gas) +	3.600	0.1066	57	0.7250 (3hr)	68	0.8250	60	0.8483	44	0.5017
Ethylene Oxide (Gas) +	0.650	0.0231	25	0.1420 (3hr)	20	0.1418	24	0.1683	32	0.1160
Hydrogen Sulfide (Gas) +	0.030	0.0008 µL	4	0.0028 (3hr)	4	0.0017	4	0.0005	4	0.0017
Hydrogen Sulfide (Gas) (27C) +	0.010	0.0003 µL	8	0.0070 (3hr)	8	0.0055	8	0.0077	8	0.0068
Hydrogen Sulfide (Gas) +	0.030	0.0008 µL	15	0.0078 (ac)	20	0.0017	12	0.0133	12	0.0083
Isoprene	0.010	0.0005	9	0.1820 (3hr)	8	0.0615	8	0.1295	12	0.3550
Methane (27C) +	1.000	0.0129	7	18.0000 (ac)	7	16.0000	6	27.0000	8	11.0000
Methyl Acetate +	0.020	0.0012	112	0.0053 (3hr)	84	0.0072	144	0.0042	108	0.0048
Methyl Acrylate +	7.000	0.4861	?	(3hr)	116	0.7683	112	0.7700	> 180	
Methyl Bromide (Gas) +	0.400	0.0306	21	0.0347 (3hr)	20	0.0367	20	0.0367	24	0.0308
Methyl Bromide (Gas) +	0.020	0.0015 µL	20	0.0065 (3hr)	20	0.0053	20	0.0073	20	0.0067
Methyl Chloride (Gas) (27C) +	0.060	0.0024 µL	16	0.0020 (as)	16	0.0020	16	0.0020	16	0.0020
Methyl Chloroformate +	0.050	0.0038	81	0.0120 (3hr)	76	0.0092	76	0.0198	92	0.0068
Methyl Chloroformate (27C) +	0.100	0.0076	95	0.9500 (3hr)	116	0.7500	72	1.2000	96	0.8900
Methyl Iodide +	0.370	0.0424	32	17.2333 (3hr)	32	27.0000	32	10.8000	32	13.9000
Methyl Isocyanate +	0.010	0.0005	92	0.0202 (3hr)	96	0.0207	72	0.0188	108	0.0212
Nitric Oxide (Gas) +	1.000	0.0508 µL	30	2.0000 (ac)						
Nitrogen Dioxide (Gas) (27C) +	0.500	0.0186 µL	4	4.9900 (as)	4	5.3333	4	6.3500	4	3.2833
Nitrogen Tetroxide (Gas) +	0.080	0.0059 µL	15	13.7600 (as)	24	16.2000	4	18.7000	16	6.4000
Nitromethane	0.730	0.0359	168	0.0538 (ac)	168	0.0447	168	0.0630	168	0.0537
Pentane +	0.010	0.0006	81	0.0440 (ac)	88	0.0500	64	0.0500	92	0.0333
Phosgene (Gas) +	0.500	•	60	3.3300 (ac)	60	3.3300	60	3.3300	60	3.3300

(Continued)

TABLE 6. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5200 AT 25C

Chemical +	MDL* (ppm)	MDR* (µg/cm²-min)	Average BT (min)	Average Reported rate** (µg/cm²-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (µg/cm²-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (µg/cm²-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (µg/cm²-min)
Propylene Oxide (27C) +	0.010	0.0005	89	0.0001 (3hr)	96	0.0001	96	0.0001	76	0.0002
Sulfur Dioxide (Gas) +	47.000	2.4292 mL	60	0.0895 (3hr)	60	0.0717	60	0.1250	60	0.0717
Sulfur Dioxide (Gas) +	1.000	0.0517 mL	40	2.3000 (ac)	30	2.3000	60	2.3000	30	2.3000
Trichloroethylene +	0.010	0.0011	49	0.1949 (3hr)	52	0.2017	56	0.1630	40	0.2200
Trichloroethylene (27C) +	0.010	0.0011	72	0.0028 (3hr)	80	0.0022	76	0.0042	60	0.0022
Trimethylamine +	0.150	0.0072	20	(ac)	20					
Trimethylamine +	0.014	0.0007	> 180							
Trimethylamine +	0.150	0.0072	25	(ac)	20		24		32	
Vinyl Acetate	0.020	0.0014	69	0.2522 (ac)	68	0.2433	64	0.3350	76	0.1783
Vinyl Acetate +	0.004	0.0003	73	38.0000 (3hr)	65	50.0000	85	35.0000	69	29.0000
Vinyl Acetate +	0.004	0.0003	109	11.2800 (3hr)	72	25.2000	132	2.1900	124	6.4400
Vinyl Chloride (Gas) +	0.010	0.0005 µL	12	0.0840 (3hr)	12	0.0860	12	0.0952	12	0.0715
Vinyl Chloride (Gas) +	0.020	0.0010 µL	7	0.0600 (3hr)	4	0.0800	8	0.0400	8	0.0400
Vinyl Methyl Ether +	33.000	1.5448	28	19.1000 (3hr)	36	7.6500	24	35.0500	24	14.6000
Vinylidene Chloride	0.490	0.0383	124	1.0828 (3hr)	120	1.4800	120	0.8800	132	0.8883
Vinylidene Chloride +	0.010	0.0008	40	0.0860 (3hr)	32	0.1570	40	0.0655	48	0.0352
Vinylidene Chloride (27C) +	0.030	0.0023	61	0.0822 (3hr)	64	0.0567	60	0.0900	60	0.1000
Vinylidene Fluoride (Gas) +	0.040	0.0021	32	0.0760 (3hr)	32	0.0700	32	0.0900	32	0.0700

+ Received after initial model development effort.

* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (*) could not be converted. ND indicates not determined.
Note: µL indicates the MDR and reported rate are in units of µL/cm²-min, mL indicates MDR and reported rate are in units mL/cm²-min.

** Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses. (ss) indicates a steady-state permeation rate value. (ac) indicates that no permeation time curve was available.

3.3.3 Comparison of Challenge 5100 with Challenge 5200 Results

As noted above, there were 39 chemicals tested against both Challenge 5100 and Challenge 5200. The results of these tests are compared in Table 7. In the broadest sense, there is good agreement between the results for the two fabrics: chemicals detected to permeate Challenge 5100 within 3 hours were also detected to permeate Challenge 5200 and vice versa. In all, there were 7 chemicals with some discrepancy. For 6 of these chemicals, the discrepancy was within one fabric (e.g., repeat test results for the same fabric conflicted, results within the 3 replicates of a test conflicted). For the remaining case (vinylidene fluoride), the results conflict, however, the MDR for the Challenge 5200 test was an order of magnitude lower than for the Challenge 5100 test.

For the remaining 32 chemicals, the results are in agreement. For 20 of these chemicals, no permeation was detected for either material. For the other 12 chemicals, permeation was detected through both materials. It is difficult, however, to make specific comparisons between the breakthrough times and reported permeation rates for these permeating chemicals because of differences in the MDRs and the test durations. In spite of these differences, the following generalizations are possible:

- the results were approximately equal for four chemicals,
- the permeation resistance was somewhat better for Challenge 5100 for seven chemicals, and
- the permeation resistance was somewhat better for Challenge 5200 for only one chemical.

Our conclusion based on this analysis is that the barrier properties of the two materials are similar. Therefore, for the purposes of predictive model development, the data set was combined and a single model developed to address both materials. Again, we also concluded that the variability in the permeation method and detection limits make the development of a quantitative predictive model difficult. Analysis of the overall data set and the development of an empirical model to predict pure chemical permeation of the Challenge materials are discussed in Section 4.

3.4 CHEMICAL MIXTURE DATA SET

Table 8 summarizes the permeation tests that were conducted with chemical mixtures at (or near) 25°C including both the TRI and Arthur D. Little tests. Compared to the data set for pure chemicals reported above, very few of the infinite number of chemical mixtures possible were tested. Consequently, only general guidelines regarding mixture permeation behavior are possible. The TRI mixture permeation test results, as compiled by us, are provided in Appendix C. The Arthur D. Little mixture permeation test results are documented in Appendix D using the ASTM F1194-89 format for reporting the results of chemical permeation testing. Both these data sets are discussed further in Section 5.

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH CHALLENGE 5100 AND 5200 AT 25°C

Chemical	Material	MDL* (ppm)	MDR* (μg/cm²-min)	Average BT (min)	Average reported rate** (μg/cm²-min)	
Acetone	5100	1.2	0.047	>210	--	
(27°C)	5200	nd	nd	70	1.6	(3hr)
		1.0	0.040	>180	--	(3hr)
(27°C)		0.010	0.0004	116	0.0004	
(27°C)		0.001	0.00004	>180	--	
(ChemFab)		0.10	•	>300	--	
Acetonitrile	5100	nd	nd	>270	--	
	5200	1.0	0.033	>180	--	
		2.0	0.066	>180	--	
Acetyl chloride	5100	35.5	2.25	>186	--	
	5200	0.020	0.0013	>180	--	
Allyl chloride	5100	0.060	0.0037	143	0.013	(ss)
		0.16	0.0099	134	0.011	(6hr)
	5200	0.030	0.0019	56	0.28	(3hr)
Ammonia gas	5100	0.040	0.0005	>180	--	
	5200	0.30	0.0041	31	0.11	(ss)
		0.070	μL 0.0010	25	0.24	(3hr)
		0.030	μL 0.0004	32	0.15	(3hr)
(ChemFab)		0.10	•	>300	--	
Ammonium hydroxide	5100	2.0	0.057	30, >180†	26.7	(3hr)
		7.2	0.20	>180	--	
	5200	0.25	0.0071	>180	--	
		7.2	0.20	120	0.34	(3hr)
Butylamine	5100	0.32	0.019	>180	--	
	5200	0.010	0.0006	>180	--	
Carbon Disulfide	5100	0.10	0.0061	20	0.050	(ss)
	5200	0.010	0.0006	20	0.034	(3hr)
(ChemFab)		0.30	•	143	0.050	(nc)
m-Cresol (Cresols)	5100	0.030	0.0026	>240	--	
	5200	0.010	0.0009	>180	--	
Dibromomethane	5100	0.050	0.0070	>180	--	
	5200	0.030	0.0042	>180	--	
1,2-Dichloroethylene	5100	0.010	0.0008	15	1.1	(ss)
		0.010	0.0008	23	0.13	(ss)
	5200	0.010	0.0008	24	0.36	(nc)

(continued)

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH CHALLENGE 5100 AND 5200 AT 25°C

Chemical	Material	MDL* (ppm)	MDR* (μg/cm²-min)	Average BT (min)	Average reported rate** (μg/cm²-min)	
Dichloromethane	5100	0.27	0.0042	51	0.020	(ss)
(USCG)		0.030	•	61	nd	(nc)
(27°C)	5200	0.007	0.0005	83	3.7	(3hr)
		0.005	0.0003	64	0.26	(3hr)
(ChemFab)		0.10	•	64	0.12	(nc)
Diethylamine (USCG)	5100	nd	nd	>270	--	
(ChemFab)	5200	0.40	•	>300	--	
Dimethylformamide (USCG)	5100	nd	nd	>192	--	
(ChemFab)	5200	0.70	•	>300	--	
Ethyl acetate	5100	0.49	0.035	>258	--	
	5200	0.010	0.0007	>180	--	
(ChemFab)		0.10	•	>300	--	
Ethyl acrylate	5100	1.7	0.14	>1020	--	
	5200	0.050	0.0040	>180	--	
Ethyl ether	5100	0.13	0.0078	>180	--	
		0.010	0.0006	92	0.005	(3hr)
(27°C)		0.006	0.0004	117	1.1	(3hr)
(27°C)	5200	0.010	0.0006	127	0.38	(20hr)
(27°C)		0.010	0.0006	92	0.0080	(3hr)
(27°C)		0.003	0.0002	149	2.1	(3hr)
(27°C)		0.010	0.0006	40	173.3	(3hr)
Ethyl vinyl ether	5100	0.030	0.0017	113	0.0080	(3hr)
	5200	0.020	0.0012	23	0.67	(3hr)
Freon 12 gas	5100	3.5	μL 0.34	160, >180†	0.0001	(3hr)
	5200	0.10	0.0098	>180	--	
Gasoline (Gasoline JP-4)	5100	1.7	•	>894	--	
	5200	0.1	•	>180	--	
Hexane	5100	0.25	0.017	>300	--	
	5200	0.10	0.0070	>300	--	
Methanol	5100	4.1	0.11	>852	--	
(ChemFab)	5200	0.40	•	>300	--	
Methyl acrylate	5100	0.12	0.0083	>180	--	
	5200	7.0	0.49	114, >180†	0.77	(3hr)
Methyl bromide gas	5100	0.010	μL 0.0008	27	0.0004	(ss)
	5200	0.40	0.031	21	0.035	(3hr)
		0.020	μL 0.0015	20	0.0065	(3hr)
Methyl ethyl ketone	5100	0.65	0.038	>180	--	
(ChemFab)	5200	1.0	•	>120	--	

(continued)

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH CHALLENGE 5100 AND 5200 AT 25°C

Chemical	Material	MDL* (ppm)	MDR* (μg/cm²-min)	Average BT (min)	Average reported rate** (μg/cm²-min)	
Methyl vinyl ketone	5100	0.050	0.0028	>180	--	
	5200	0.010	0.0006	>180	--	
Nitrobenzene	5100	0.080	0.0079	>180	--	
(ChemFab)	5200	1.0	*	>300	--	
Nitromethane	5100	0.26	0.013	>180	--	
	5200	0.73	0.036	168	0.054	(nc)
		0.70	0.035	>180	--	
Potassium hydroxide	5100	1.0	0.045	>180	--	
	5200	0.50	0.023	>180	--	
Propylene oxide	5100	0.68	0.0080	154	0.021	(ss)
(27°C)	5200	0.010	0.0005	89	0.0002	(3hr)
Sodium hydroxide (50%)	5100	0.50	0.016	>4260	--	
(USCG)		nd	nd	>180	--	
	5200	0.50	0.016	>180	--	
(ChemFab)		0.20	*	>300	--	
Tetrachloroethylene	5100	0.11	0.015	>624	--	
(USCG)		nd	nd	103	nd	
(27°C)		0.001	0.0001	26, >180†	18.0	(3hr)
(ChemFab)	5200	0.20	*	>300	--	
Tetrahydrofuran (USCG)	5100	nd	nd	>330	--	
(ChemFab)	5200	0.10	*	>300	--	
Toluene	5100	0.060	0.0045	>180	--	
(ChemFab)	5200	0.10	*	>300	--	
Trichloroethylene	5100	0.070	0.0017	148	0.031	(ss)
		0.010	0.0011	138	0.031	(6hr)
	5200	0.010	0.0011	49	0.19	(3hr)
		0.010	0.0011	72	0.0028	(3hr)
Vinyl acetate	5100	0.21	0.0036	106	0.059	(ss)
	5200	0.020	0.0014	69	0.25	(nc)
		0.004	0.0003	73	38.0	(3hr)
		0.004	0.0003	109	11.3	(3hr)
Vinyl methyl ether	5100	0.54	0.025	60	2.2	(3hr)
	5200	33.0	1.5	28	19.1	(3hr)

(continued)

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH CHALLENGE 5100 AND 5200 AT 25°C

Chemical	Material	MDL* (ppm)	MDR* (μg/cm²-min)	Average BT (min)	Average reported rate** (μg/cm²-min)	
Vinylidene chloride	5100	0.49	0.038	>180	--	
		0.010	0.0008	51	0.022	(3hr)
	5200	0.49	0.038	124	1.1	(3hr)
		0.010	0.0008	40	0.086	(3hr)
		0.030	0.0023	61	0.082	(3hr)
Vinylidene fluoride	5100	0.70	0.036	>180	--	
	5200	0.040	0.0021	32	0.076	(3hr)

* MDL = minimum detectable concentration determined by syringe pump calibration; MDR = minimum detectable permeation rate calculated from MDL, carrier gas flowrate, and material surface area. Values entered as (*) could not be converted, (nd) indicates not determined, and μL indicates values reported as μL instead of μg.

** Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value, and (nc) indicates that no permeation time curve was provided.

† Conflicting results were measured within the three replicates for this test.

TABLE 8. SUMMARY OF MIXTURE PERMEATION TESTS AT 25°C

Condition	No. of mixtures	
	TRI	Arthur D. Little
Total mixtures tested against Challenge 5100 material	15	--
- Binary mixtures	14	--
- Ternary mixtures	1	
- Tests for which permeation rates as a function of time were measured	0	--
Total mixtures tested against Challenge 5200 material	14	7
- Binary mixtures	10	5
- Ternary mixtures	4	2
- Tests for which permeation rates as a function of time were measured	0	7

SECTION 4

DEVELOPMENT OF A MODEL TO PREDICT PURE CHEMICAL PERMEATION

4.1 FICK'S LAW ANALYSIS

Our first step in analyzing the data set was to assess the mechanism by which the chemicals permeate the Challenge materials as a function of time. Such an assessment is important because the direction and success of predictive model development often depend on the permeation mechanism. For example, if the permeation appears to be a solution-diffusion process, then a Fick's law model can be pursued and the permeation behavior as a function of time can be predicted using theoretical relationships. If the mechanism is not solution-diffusion (e.g., analogous to an inert gas penetrating a film or microporous substrate), then a more empirical model might be pursued to predict whether permeation will occur.

4.1.1 Analysis of Permeation-Time Behavior

The available permeation-time curves were analyzed to assess whether the behavior could be accurately described by a solution-diffusion mechanism using Fick's laws of diffusion [11]. Mathematical relationships based on Fick's law describe the permeation rate, J, and the cumulative amount permeated, M, at any time following initiation of chemical contact for solution-diffusion processes. These relationships require two fundamental parameters: the diffusion coefficient, D, and the solubility, S, of the permeant in the material of interest. For a planar film of thickness, l, the appropriate solutions to Fick's second law of diffusion with standard initial conditions and simple boundary conditions are:

$$J=(DS/l)[1+2\sum_{n=1}^{\infty}(-1)^n\exp(-\pi^2n^2\psi)] \qquad \text{Eq. (1)}$$

and

$$M = (Sl)[\psi-1/6-2\sum_{n=1}^{\infty}[(-1)^n/(\pi n)^2]\exp(-(n\pi)^2\psi)] \qquad \text{Eq. (2)}$$

where J = permeation rate, $\mu g/cm^2$-min
M = cumulative amount permeated, $\mu g/cm^2$
ψ = Dt/l^2, dimensionless
D = diffusion coefficient, cm^2/min

S	=	equilibrium solubility, $\mu g/cm^3$
l	=	membrane thickness, cm
t	=	time, min

The derivation of these equations assumes that there is continuous contact of the chemical with the clothing material surface for the test duration, there are no external resistances at the clothing material surfaces, and the diffusion coefficient and clothing material thickness are constants. The last assumption is not always valid and, particularly for rubbery polymer systems, the concentration dependence of D and swelling must be considered for accurate predictions of the permeation behavior.

Using these equations, one can calculate values for the breakthrough time on the basis of a minimum detectable permeation rate or a minimum cumulative amount permeated. These equations can also be used to solve for values of D and S given a set of J versus t or M versus t data [12]. For this data set, the permeation-time curves provide sets of J versus t data that can also be converted to M versus t data by analysis of the areas under the permeation-time curves as a function of time. Two approaches to extract values for D and S were pursued depending on the type of curve available. For permeation curves in which steady-state was reached, values for D and S were solved for directly by converting the later time data (i.e., steady-state data) to cumulative amounts permeated and applying Eq. (2). For permeation-time curves in which permeation rates were still increasing with time (i.e., in the transition region of a Fickian permeation curve), values for D and S were determined using Eq. (1) and an iterative curve-fitting technique. Both techniques are described in Appendix E.

Once values for D and S were determined, Eq. (1) was used to calculate permeation rates as a function of time for comparison with the reported permeation data. In general, the measured permeation-time curves could be accurately described using the Fick's law model. Figure 1 shows an example curve fit for a case in which the permeation rate data reached steady-state. A second example is shown in Figure 2 for a test that was terminated before reaching steady-state. Figure 2 also illustrates an important capability of this analysis technique that can simplify data comparisons. With the values of D and S and Eq. (1), the permeation behavior at any time can be calculated, including the steady-state permeation rate and the time required to reach steady-state. Thus, permeation results from different tests can be more readily compared by calculating a permeation rate at a set test duration or by calculating the steady-state permeation rate.

Values for D, S, and the steady-state permeation rate calculated using Eq. (1) are reported in Table 9 for Challenge 5100 at 25°C, Table 10 for Challenge 5200 at 25°C, Table 11 for Challenge 5200 at 35°C, and Table 12 for Challenge 5200 at 40°C. Analyses were not possible for the 30°C data because permeation-time curves were not provided to us for that data set.

In general, an excellent fit to the permeation data was possible using Fick's law with the assumption of a constant D. As reported in Tables 9 through 12, the D values ranged from 10^{-10} to 10^{-9} cm^2/s. These values are quite low compared to other protective clothing polymers, particularly elastomers, that have typical values in the range from

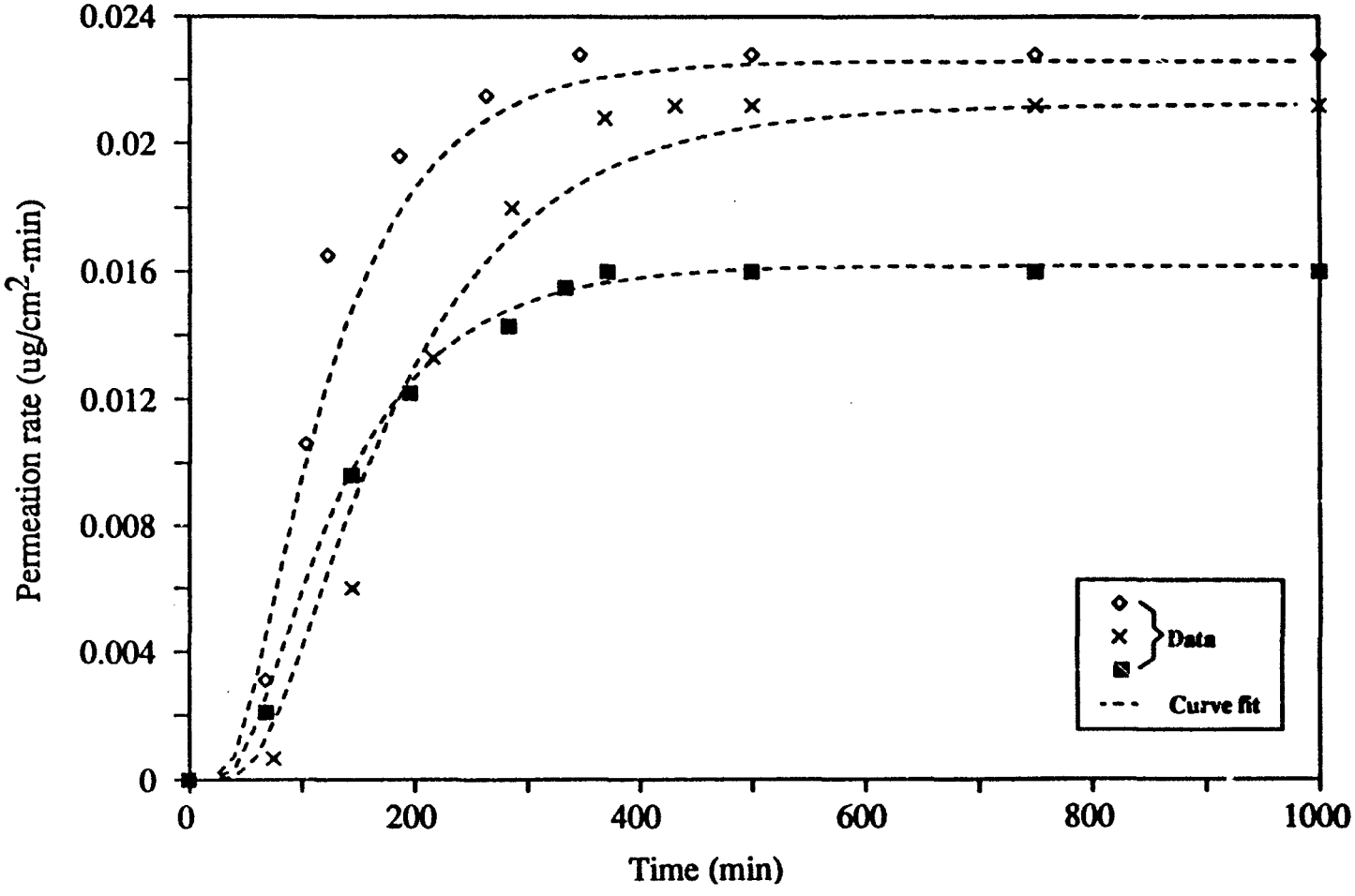


Figure 1. Fick's law curve fit for dichloromethane permeation through Challenge 5100 at 25°C. (D_{ave}= 1.1 x 10^{-9} cm^2/s, S_{ave}= 2.4 x 10^{-3} g/cm^3, l = 0.008 cm)

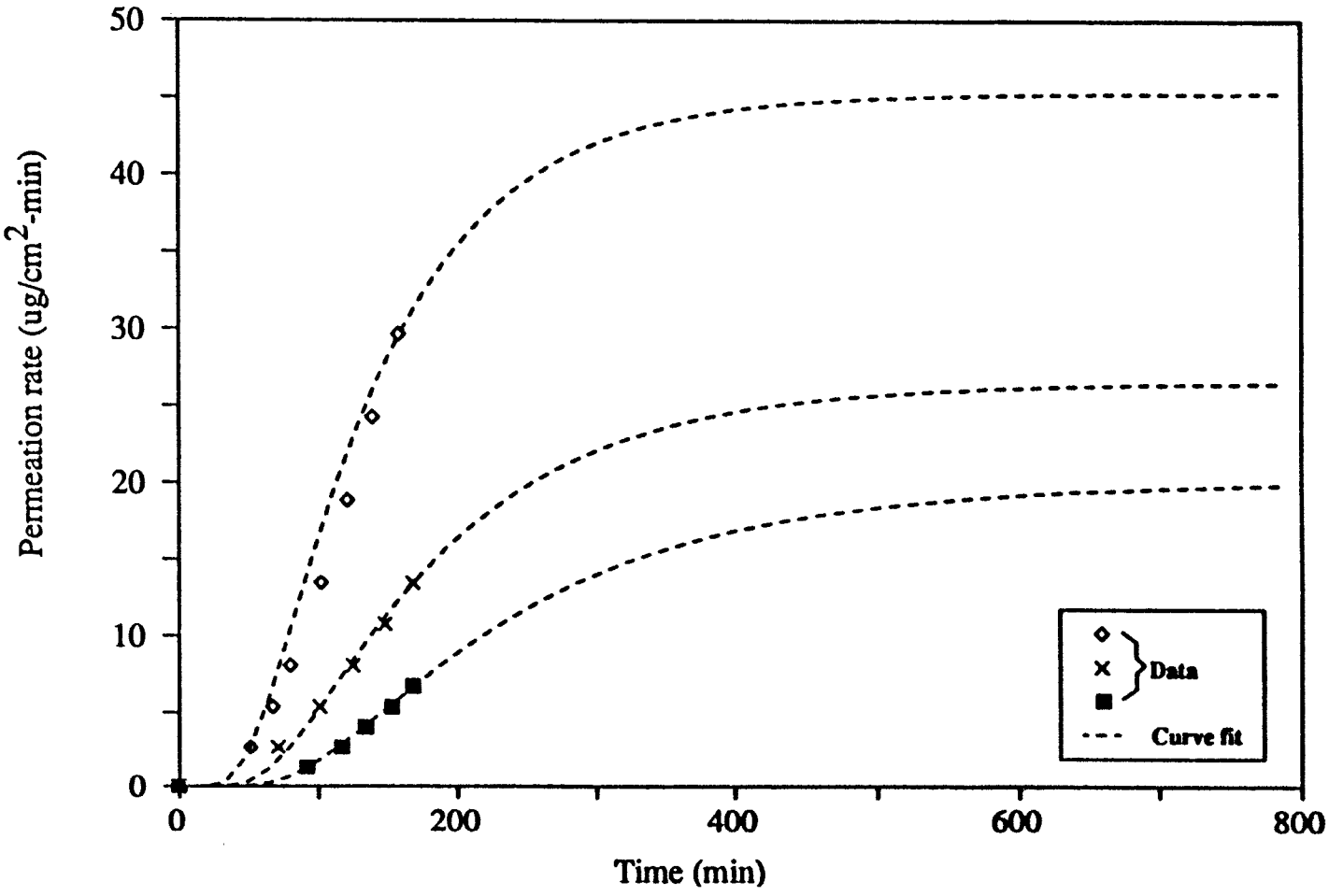


Figure 2. Fick's law curve fit for vinyl methyl ether permeation through Challenge 5200 at 25°C. (D_{ave}= 9.2 x 10^{-10} cm^2/s, S_{ave}= 4.4 g/cm^3, l = 0.008 cm)

TABLE 9. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5100 AT 25°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Allyl Chloride	136	0.010	2.2×10^{-10}	2.7×10^{-10}	4.6×10^{-2}	3.8×10^{-2}	0.073
	116	0.021	3.6×10^{-10}		1.8×10^{-2}		0.049
	176	0.007	2.2×10^{-10}		4.9×10^{-2}		0.070
	166	0.010	1.8×10^{-10}	1.8×10^{-10}	7.7×10^{-3}	7.7×10^{-3}	0.010
Carbon Disulfide	18	0.043	3.0×10^{-9}	2.8×10^{-9}	1.9×10^{-3}	2.7×10^{-3}	0.043
	21	0.061	3.9×10^{-9}		2.1×10^{-3}		0.061
	22	0.046	1.5×10^{-9}		4.0×10^{-3}		0.046
Chloroprene	192	0.003	5.7×10^{-10}	5.8×10^{-10}	6.2×10^{-4}	1.1×10^{-3}	0.003
	184	0.003	6.4×10^{-10}		7.0×10^{-4}		0.003
	160	0.009	5.3×10^{-10}		2.1×10^{-3}		0.008
Dichloroethylene	21	0.14	1.8×10^{-9}	1.6×10^{-9}	9.3×10^{-3}	1.1×10^{-2}	0.12
	24	0.12	1.3×10^{-9}		1.3×10^{-2}		0.12
Dichloromethane	47	0.023	1.3×10^{-9}	1.1×10^{-9}	2.3×10^{-3}	2.4×10^{-3}	0.023
	50	0.016	1.2×10^{-9}		1.8×10^{-3}		0.016
	55	0.021	8.9×10^{-10}		3.2×10^{-3}		0.021
Ethyl Ether	88	0.006	3.8×10^{-10}	3.9×10^{-10}	2.4×10^{-2}	2.0×10^{-2}	0.069
	84	0.008	3.8×10^{-10}		3.1×10^{-2}		0.089
	104	0.001	4.0×10^{-10}		4.5×10^{-3}		0.013
Ethyl Vinyl Ether	148	0.004	8.9×10^{-10}	1.3×10^{-9}	1.2×10^{-1}	1.1×10^{-1}	0.77
	92	0.012	1.7×10^{-9}		1.0×10^{-1}		1.3
	100	0.008	1.4×10^{-9}		1.0×10^{-1}		1.1

(continued)

TABLE 9. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5100 AT 25°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Methyl Bromide (Gas)	6	ul 0.0002	2.5×10^{-9}	2.1×10^{-9}	1.2×10^{-5}	2.9×10^{-5}	0.0002
	11	0.0005	1.8×10^{-9}		3.4×10^{-5}		0.001
	12	0.0005	1.9×10^{-9}		4.1×10^{-5}		0.001
Propylene (Gas)	60	0.0002	1.7×10^{-9}	1.8×10^{-9}	2.2×10^{-5}	2.7×10^{-5}	0.0003
	48	0.001	2.0×10^{-9}		3.8×10^{-5}		0.001
	76	0.0002	1.7×10^{-9}		2.2×10^{-5}		0.0006
Propylene Oxide	170	0.018	2.9×10^{-10}	2.9×10^{-10}	1.1×10^{-2}	1.1×10^{-2}	0.024
Trichloroethylene	143	0.034	4.2×10^{-10}	4.1×10^{-10}	1.1×10^{-2}	1.0×10^{-2}	0.034
	156	0.027	3.9×10^{-10}		9.4×10^{-3}		0.027
Vinyl Acetate	74	0.055	5.6×10^{-10}	5.1×10^{-10}	1.3×10^{-2}	1.6×10^{-2}	0.055
	137	0.062	4.6×10^{-10}		1.8×10^{-2}		0.062
Vinyl Methyl Ether	60	3.6	7.8×10^{-10}	8.3×10^{-10}	1.4	8.3×10^{-1}	8.1
	60	2.4	7.7×10^{-10}		9.2×10^{-1}		5.3
	60	0.78	9.3×10^{-10}		1.8×10^{-1}		1.3
Vinylidene Chloride	52	0.012	6.2×10^{-10}	6.3×10^{-10}	7.6×10^{-3}	1.2×10^{-2}	0.036
	52	0.011	6.2×10^{-10}		7.6×10^{-3}		0.036
	48	0.043	6.4×10^{-10}		2.2×10^{-2}		0.11

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 25°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Allyl Chloride	68	0.29	5.9×10^{-10}	5.3×10^{-10}	1.5×10^{-1}	2.8×10^{-1}	0.69
	64	0.15	4.5×10^{-10}		2.5×10^{-1}		0.87
	36	0.41	5.5×10^{-10}		4.2×10^{-1}		1.7
Ammonia (Gas)	36	0.078	2.4×10^{-9}	3.2×10^{-9}	4.3×10^{-3}	4.6×10^{-3}	0.076
	24	0.16	3.6×10^{-9}		5.7×10^{-3}		0.16
	32	0.11	3.6×10^{-9}		3.7×10^{-3}		0.099
	32	µL 0 12	1.7×10^{-9}	1.8×10^{-9}	1.4×10^{-2}	1.6×10^{-2}	0.17
	32	0.22	1.8×10^{-9}		2.2×10^{-2}		0.29
	32	0.11	1.9×10^{-9}		1.3×10^{-2}		0.19
Bromochloromethane	93	0.019	6.2×10^{-10}	5.8×10^{-10}	5.0×10^{-3}	5.5×10^{-3}	0.023
	109	0.015	5.2×10^{-10}		5.0×10^{-3}		0.019
	93	0.023	6.0×10^{-10}		6.4×10^{-3}		0.029
Bromoethane	144	0.024	2.9×10^{-10}	4.1×10^{-10}	1.5×10^{-1}	8.9×10^{-2}	0.032
	84	0.032	5.8×10^{-10}		2.8×10^{-2}		0.12
	132	0.027	3.5×10^{-10}		8.8×10^{-2}		0.23
1,3-Butadiene (Gas)	24	µL 0.13	1.1×10^{-9}	1.2×10^{-9}	2.4×10^{-2}	1.3×10^{-2}	0.20
	24	0.070	1.1×10^{-9}		1.1×10^{-2}		0.097
	24	0.038	1.3×10^{-9}		4.9×10^{-3}		0.048
	8	0.024	9.8×10^{-10}	1.0×10^{-9}	4.1×10^{-3}	6.2×10^{-3}	0.030
	4	0.038	9.5×10^{-10}		6.8×10^{-3}		0.048
	4	0.055	1.1×10^{-9}		7.6×10^{-3}		0.062

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 25°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
1-Chloropropane	269	0.24	2.1×10^{-10}	2.4×10^{-10}	8.6×10^{-1}	6.8×10^{-1}	1.3
	225	0.33	2.7×10^{-10}		4.9×10^{-1}		0.98
cis-1,2-Dichloroethylene	56	0.22	4.4×10^{-10}	3.6×10^{-10}	5.3×10^{-1}	7.2×10^{-1}	1.7
	80	0.097	2.9×10^{-10}		9.4×10^{-1}		2.0
	72	0.15	3.4×10^{-10}		6.8×10^{-1}		1.7
trans-1,2-Dichloroethylene	19	1.4	9.8×10^{-10}	1.1×10^{-9}	2.2×10^{-1}	2.0×10^{-1}	1.6
	19	1.5	1.1×10^{-9}		2.0×10^{-1}		1.6
	19	1.3	1.1×10^{-9}		1.7×10^{-1}		1.4
Dichloromethane	68	0.23	5.4×10^{-10}	5.7×10^{-10}	2.2×10^{-1}	2.3×10^{-1}	0.90
	52	0.37	6.7×10^{-10}		1.8×10^{-1}		0.94
	72	0.19	4.9×10^{-10}		2.6×10^{-1}		0.95
(27°C)	84	4.0	4.9×10^{-10}	5.1×10^{-10}	5.8	5.3	21.1
	88	3.0	5.7×10^{-10}		3.5		14.9
	76	4.0	4.5×10^{-10}		6.7		22.5
Dimethyl Sulfide	116	0.0005	3.5×10^{-10}	4.8×10^{-10}	10.2	4.8	26.1
	76	0.0005	4.8×10^{-10}		3.0		10.5
	92	0.0005	6.0×10^{-10}		1.3		5.8

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 25°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Ethylene Oxide (Gas)	68	0.83	$7.1x10^{-10}$	$9.0x10^{-10}$	$4.1x10^{-1}$	$2.7x10^{-1}$	2.0
	60	0.85	$7.8x10^{-10}$		$3.3x10^{-1}$		1.8
	44	0.50	$1.2x10^{-9}$		$7.2x10^{-2}$		0.66
	20	0.14	$1.7x10^{-9}$	$1.5x10^{-9}$	$1.1x10^{-2}$	$1.4x10^{-2}$	0.14
	24	0.17	$1.5x10^{-9}$		$1.9x10^{-2}$		0.14
	32	0.12	$1.4x10^{-9}$		$1.2x10^{-2}$		0.13
Ethyl Ether	104	0.41	$3.8x10^{-10}$	$3.4x10^{-10}$	$1.3x10^{-1}$	$1.4x10^{-1}$	0.36
	136	0.30	$3.2x10^{-10}$		$1.3x10^{-1}$		0.31
	140	0.42	$3.3x10^{-10}$		$1.5x10^{-1}$		0.65
Ethyl Vinyl Ether	40	0.39	$5.0x10^{-10}$	$5.3x10^{-10}$	$4.8x10^{-1}$	$6.4x10^{-1}$	1.8
	8	0.55	$4.6x10^{-10}$		$7.9x10^{-1}$		2.7
	20	1.1	$6.4x10^{-10}$		$6.6x10^{-1}$		3.2
Hydrogen Sulfide (Gas)	8	µL 0.0055	$4.7x10^{-9}$	$5.0x10^{-9}$	$1.5x10^{-4}$	$1.7x10^{-4}$	0.0054
	8	0.0077	$6.0x10^{-9}$		$1.7x10^{-4}$		0.0076
	8	0.0068	$4.3x10^{-9}$		$2.0x10^{-4}$		0.0066
Isoprene	8	0.062	$4.2x10^{-9}$	$4.6x10^{-9}$	$8.6x10^{-2}$	$5.1x10^{-2}$	2.7
	8	0.13	$8.2x10^{-9}$		$3.2x10^{-2}$		1.9
	12	0.36	$1.5x10^{-9}$		$3.4x10^{-2}$		3.8
Methyl Acetate	84	0.007	$4.8x10^{-10}$	$5.0x10^{-10}$	$1.2x10^{-2}$	$8.7x10^{-3}$	0.040
	144	0.004	$4.2x10^{-10}$		$1.0x10^{-2}$		0.028
	108	0.005	$6.0x10^{-10}$		$4.2x10^{-3}$		0.018

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 25°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Methyl Bromide (Gas)	20	µL 0.005	$1.7x10^{-9}$	$1.7x10^{-9}$	$4.1x10^{-4}$	$5.3x10^{-4}$	0.006
	20	0.007	$1.9x10^{-9}$		$5.6x10^{-4}$		0.008
	20	0.007	$1.5x10^{-9}$		$6.3x10^{-4}$		0.007
	20	0.037	$2.3x10^{-9}$	$2.2x10^{-9}$	$2.5x10^{-3}$	$2.5x10^{-3}$	0.042
	20	0.037	$2.1x10^{-9}$		$2.6x10^{-3}$		0.041
	20	0.031	$2.1x10^{-9}$		$2.3x10^{-3}$		0.036
Methyl Iodide	32	27.0	$1.0x10^{-9}$	$8.2x10^{-10}$	4.8	5.1	35.3
	32	10.8	$6.7x10^{-10}$		6.0		21.7
	32	13.9	$8.0x10^{-10}$		4.6		43.4
Methyl Isocyanate	96	0.021	$2.1x10^{-9}$	$2.0x10^{-9}$	$1.4x10^{-3}$	$1.4x10^{-3}$	0.022
	72	0.019	$2.0x10^{-9}$		$1.3x10^{-3}$		0.019
	108	0.021	$1.9x10^{-9}$		$1.6x10^{-3}$		0.023
Nitrogen Dioxide (Gas)	4	µL 5.3	$5.5x10^{-9}$	$4.0x10^{-9}$	$1.2x10^{-1}$	$1.8x10^{-1}$	5.0
	4	6.4	$3.3x10^{-9}$		$2.7x10^{-1}$		6.7
	4	3.3	$3.1x10^{-9}$		$1.4x10^{-1}$		3.3
Propylene Oxide	96	0.00008	$4.2x10^{-10}$	$5.3x10^{-10}$	$2.1x10^{-4}$	$1.3x10^{-4}$	0.00064
	96	0.00007	$5.4x10^{-10}$		$6.1x10^{-5}$		0.00025
	76	0.0002	$6.2x10^{-10}$		$1.3x10^{-4}$		0.00061
Trichloroethylene	52	0.20	$4.3x10^{-10}$	$3.6x10^{-10}$	$3.5x10^{-1}$	$7.2x10^{-1}$	1.1
	56	0.16	$2.9x10^{-10}$		$6.2x10^{-1}$		1.3
	40	0.22	$3.6x10^{-10}$		1.2		3.2

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 25°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Vinyl Acetate	65	50.0	4.9×10^{-10}	4.7×10^{-10}	74.8	80.3	271.1
	85	35.0	3.8×10^{-10}		136.7		392.9
	69	29.0	5.4×10^{-10}		29.3		117.3
	72	25.2	2.2×10^{-10}	2.2×10^{-10}	2354.1	1084.9	3824.4
	132	2.2	2.2×10^{-10}		203.2		330.1
	124	6.4	2.2×10^{-10}		697.3		1045.9
Vinyl Chloride (Gas)	12	µL 0.15	2.7×10^{-9}	1.9×10^{-9}	9.0×10^{-1}	1.4	18.1
	12	0.16	1.7×10^{-9}		1.6		20.5
	12	0.12	1.4×10^{-9}		1.7		17.6
Vinyl Methyl Ether	36	7.7	6.8×10^{-10}	9.2×10^{-10}	4.0	4.4	19.8
	24	35.1	1.2×10^{-9}		5.1		45.3
	24	14.6	8.9×10^{-10}		4.0		26.5
Vinylidene Chloride	120	1.5	5.0×10^{-10}	4.5×10^{-10}	2.1	2.6	7.7
	120	0.88	4.0×10^{-10}		4.0		11.6
	132	0.89	4.4×10^{-10}		1.8		5.7
	64	0.057	5.0×10^{-10}	5.4×10^{-10}	8.3×10^{-2}	9.0×10^{-2}	0.31
	60	0.090	6.0×10^{-10}		7.0×10^{-2}		0.30
	60	0.10	5.2×10^{-10}		1.2×10^{-1}		0.48

TABLE 11 SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 35°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Acetone	32	0.016	$7.5x10^{-10}$	$6.6x10^{-10}$	$4.4x10^{-3}$	$5.3x10^{-3}$	0.025
	80	0.014	$6.1x10^{-10}$		$5.8x10^{-3}$		0.026
	88	0.014	$6.1x10^{-10}$		$5.8x10^{-3}$		0.026
Acrylonitrile	93	0.085	$7.0x10^{-10}$	$5.8x10^{-10}$	$4.5x10^{-2}$	$6.0x10^{-2}$	0.24
	117	0.067	$5.4x10^{-10}$		$6.2x10^{-2}$		0.25
	121	0.060	$5.0x10^{-10}$		$7.3x10^{-2}$		0.28
Carbon Disulfide	12	0.61	$2.1x10^{-9}$	$2.2x10^{-9}$	$4.0x10^{-2}$	$3.3x10^{-2}$	0.62
	16	0.64	$2.5x10^{-9}$		$3.4x10^{-2}$		0.65
	20	0.44	$2.0x10^{-9}$		$2.6x10^{-2}$		0.38
Dichloromethane	44	0.22	$1.1x10^{-9}$	$1.2x10^{-9}$	$3.7x10^{-2}$	$3.1x10^{-2}$	0.32
	40	0.18	$1.3x10^{-9}$		$2.4x10^{-2}$		0.24
	44	0.17	$1.1x10^{-9}$		$3.3x10^{-2}$		0.28
Ethyl Acetate	152	0.004	$5.6x10^{-10}$	$5.8x10^{-10}$	$1.3x10^{-3}$	$1.2x10^{-3}$	0.005
	204	0.003	$4.6x10^{-10}$		$1.5x10^{-3}$		0.005
	180	0.004	$7.3x10^{-10}$		$8.0x10^{-4}$		0.004
Propylene Oxide	88	0.060	$7.8x10^{-10}$	$6.2x10^{-10}$	$2.3x10^{-2}$	$4.6x10^{-2}$	0.13
	124	0.040	$4.5x10^{-10}$		$9.5x10^{-2}$		0.32
	120	0.030	$6.4x10^{-10}$		$1.9x10^{-2}$		0.091
Tetrachloroethylene	236	0.058	$6.0x10^{-10}$	$6.8x10^{-10}$	$2.3x10^{-2}$	$1.9x10^{-2}$	0.10
	236	0.072	$8.5x10^{-10}$		$1.6x10^{-2}$		0.10
	236	0.043	$6.0x10^{-10}$		$1.7x10^{-2}$		0.076

(continued)

TABLE 11. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 35°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Trichloroethylene	68	0.33	3.4×10^{-10}	3.9×10^{-10}	1.6	1.2	4.2
	84	0.48	3.8×10^{-10}		1.2		3.5
	76	0.35	4.6×10^{-10}		6.9×10^{-1}		2.4
Vinyl Acetate	52	0.64	7.9×10^{-10}	7.3×10^{-10}	1.6×10^{-1}	1.7×10^{-1}	0.95
	52	0.84	7.7×10^{-10}		2.3×10^{-1}		1.3
	76	0.36	6.2×10^{-10}		1.2×10^{-1}		0.56

TABLE 12. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR CHALLENGE 5200 AT 40°C

Chemical	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	Average D (cm^2/s)	S (g/cm^3)	Average S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Allyl Chloride	64	0.55	$1.0x10^{-9}$	$8.6x10^{-10}$	$1.1x10^{-1}$	$1.4x10^{-1}$	0.86
	88	0.52	$8.3x10^{-10}$		$1.5x10^{-1}$		0.95
	84	0.47	$7.6x10^{-10}$		$1.6x10^{-1}$		0.90
Epichlorohydrin	132	0.25	$3.7x10^{-10}$	$3.4x10^{-10}$	1.2	1.3	3.2
	140	0.23	$3.7x10^{-10}$		$9.1x10^{-1}$		2.5
	176	0.19	$2.8x10^{-10}$		1.9		3.7
Ethyl Chloroformate	116	0.19	$4.4x10^{-10}$	$4.9x10^{-10}$	$3.1x10^{-1}$	$2.5x10^{-1}$	1.0
	104	0.22	$5.1x10^{-10}$		$2.2x10^{-1}$		0.84
	104	0.21	$5.1x10^{-10}$		$2.2x10^{-1}$		0.84
Dichloromethane	28	0.30	$1.6x10^{-9}$	$1.6x10^{-9}$	$3.0x10^{-2}$	$2.7x10^{-2}$	0.35
	32	0.23	$1.5x10^{-9}$		$2.2x10^{-2}$		0.25
	28	0.27	$1.6x10^{-9}$		$2.8x10^{-2}$		0.33
Trichloroethylene	68	0.45	$5.1x10^{-10}$	$4.8x10^{-10}$	$1.2x10^{-1}$	$1.3x10^{-1}$	0.46
	80	0.57	$5.1x10^{-10}$		$1.4x10^{-1}$		0.54
	96	0.41	$4.1x10^{-10}$		$1.4x10^{-1}$		0.42
Vinyl Acetate	68	0.24	$6.7x10^{-10}$	$6.5x10^{-10}$	$4.6x10^{-2}$	$4.9x10^{-2}$	0.23
	64	0.34	$6.8x10^{-10}$		$6.0x10^{-2}$		0.31
	76	0.18	$6.0x10^{-10}$		$4.0x10^{-2}$		0.18

10^{-8} to 10^{-6} cm^2/s. The range of values for the Challenge materials is fairly narrow but this is not unexpected because most of the chemicals analyzed are similar in size with molecular weights ranging from 50 to 150 daltons. The S values ranged from 0.0001 to 10 g/cm^3, with most values within 0.001 to 0.1 g/cm^3. Again, the majority of the S values are quite low compared to typical solubilities of these chemicals in rubber materials. Several S values, however, are surprisingly high (e.g., >1.0 g/cm^3) and raise questions regarding the Fick's law curve fitting technique as well as the accuracy of certain data sets. Possibly some of the S values should be confirmed by long-term immersion tests.

An important consequence of the generally low D and S values (and the correspondingly low permeation rates), is that the chemicals permeate the fluoropolymer material with minimal effects on the material (e.g, swelling) so that the behavior can be accurately described by an ideal Fickian solution-diffusion model.

4.1.2 Temperature Dependence

Knowledge of the effect of temperature on the permeation resistance of a protective material is critical, particularly regarding chemical protective clothing. Although permeation resistance is generally evaluated at 20-25°C, the clothing when worn will be exposed to body temperatures and environments that exceed 25°C. Some polymeric materials are relatively unaffected by temperature changes, while many are strongly affected and show a great decrease in barrier properties with small increases in temperature. Typically, the temperature dependence shows an Arrehnius relationship or exponentional change with temperature. As reported in Table 2, permeation tests were conducted for several chemicals at 30°, 35°, and 40°C. The results of these tests are summarized in Table 13 using the average breakthrough times and the average reported permeation rates. Again, because of differences in MDLs and test durations, it is difficult to directly compare many of these results. General observations on the data follow. Some chemicals that were not detected to breakthrough at 25°C were found to permeate at the higher temperatures (e.g., acetone, ethyl acetate, ethyl chloroformate). There are several cases in which the breakthrough times are shorter and permeation rates higher as temperature was increased. However, there are also several cases in which the reported breakthrough times are longer and the permeation rates are lower at the higher temperatures. We know of no explanation for such data and recommend that the tests be repeated.

The effect of temperature on the permeation behavior can also be evaluated through comparison of the D, S, and calculated steady-state permeation rate values listed in Tables 9 through 12. Use of these values may eliminate some of the data set/test method inconsistencies. Table 14 summarizes the reported permeation data and the Fick's law parameters for the 6 chemicals that were tested at three or more temperatures. These data also indicate several temperature effects: in some cases the Fick's law parameters and calculated steady-state permeation rates increase with increasing temperature, several show little or no effect, and one (vinyl acetate) shows improved permeation resistance with increasing temperature. These results are illustrated in Figures 3 through 5, in which the logarithm of the values for D (Figure 3), S (Figure 4), and calculated steady-state rate (Figure 5) are plotted versus the inverse of the absolute temperature (K). If the data followed

TABLE 13. COMPARISON OF CHALLENGE 5200 PERMEATION DATA AS A FUNCTION OF TEMPERATURE

Chemical	25°C			30°C			35°C			40°C		
	MDR*	Ave. BT (min)	Ave. reported rate** ($\mu g/cm^2$-min)	MDR	Ave. BT (min)	Ave. reported rate ($\mu g/cm^2$-min)	MDR	Ave. BT (min)	Ave. reported rate ($\mu g/cm^2$-min)	MDR	Ave. BT (min)	Ave. reported rate ($\mu g/cm^2$-min)
Acetone	0.040	>180		0.0004	>210		0.0004	67	0.015 (4hr)			
Acrolein				0.0077	56	0.095 (nc)	0.0018	23	0.068 (4hr)			
Acrylonitrile				0.0017	76	0.028 (nc)	0.0086	110	0.071 (3hr)			
Allyl chloride	0.0019	56	0.28 (3hr)	0.0031	56	0.035 (nc)	0.0080	236	0.53 (7hr)	0.0043	79	0.51 (3hr)
Carbon disulfide	0.0006	20	0.034 (3hr)	0.0006	15	0.23 (nc)	0.0006	16	0.56 (3hr)			
Dichloromethane	0.0003	64	0.26 (3hr)	0.0007	43	0.037 (nc)	0.0027	43	0.19 (3hr)	0.0021	29	0.27 (3hr)
(27°C)	0.0005	83	3.7 (3hr)									
Diethylamine				0.0024	>1182		0.0041	>180				
Dimethylformamide				0.0012	>240		0.0006	>180				
Ethyl acetate	0.0007	>180		0.0014	>300		0.0007	179	0.003 (6hr)			
Ethyl chloroformate	0.018	>180								0.0009	108	0.26 (3hr)
Hexane	0.0070	>300		0.0070	>300		0.0014	>180				
Methanol				0.0065	>300		0.016	88	0.063 (nc)			
Nitrobenzene				0.0099	>180		0.0070	>180		0.0020	>180	
Propylene oxide	0.0005	89	0.001 (3hr)	0.0005	115	0.003 (3hr)	0.0028	111	0.043 (3hr)			
Tetrachloroethylene				0.0013	>240		0.0013	236	0.058 (4hr)	0.0013	201	0.097 (3hr)
Tetrahydrofuran				0.011	>276		0.024	>180				
Toluene				0.0007	>300		0.0007	>180				
Trichloroethylene	0.0011	49	0.19 (3hr)	0.0011	84	0.14 (nc)	0.0011	76	0.34 (3hr)	0.0011	81	0.48 (ss)
	0.0011	72	0.003 (3hr)									

(continued)

TABLE 13. COMPARISON OF CHALLENGE 5200 PERMEATION DATA AS A FUNCTION OF TEMPERATURE

Chemical	25°C			30°C			35°C			40°C		
	MDR*	Ave. BT (min)	Ave. reported rate** ($\mu g/cm^2$-min)	MDR	Ave. BT (min)	Ave. reported rate ($\mu g/cm^2$-min)	MDR	Ave. BT (min)	Ave. reported rate ($\mu g/cm^2$-min)	MDR	Ave. BT (min)	Ave. reported rate ($\mu g/cm^2$-min)
Vinyl acetate	0.0030	73	38.0 (3hr)	0.0021	101	0.089 (nc)	0.0007	60	0.61 (4hr)	0.0014	69	0.25 (8hr)
	0.0030	109	11.3 (3hr)									
	0.0014	69	0.25 (nc)									

* Minimum detectable permeation rate ($\mu g/cm^2$-min)

** Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value, and (nc) indicates that no permeation time curve was provided.

TABLE 14. TEMPERATURE DEPENDENCE OF CHEMICAL PERMEATION THROUGH CHALLENGE 5200

Chemical	Temp. (°C)	MDR ($\mu g/cm^2$-min)	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Allyl Chloride	25	0.0019	56	0.28	5.3×10^{-10}	2.8×10^{-1}	1.1
	30	0.0031	56	0.035	(nc)*	(nc)	(nc)
	35	0.0080	236	0.53			
	40	0.0043	79	0.51	8.6×10^{-10}	1.4×10^{-1}	0.90
Carbon Disulfide	25	0.0006	20	0.034			
	30	0.0006	15	0.23	(nc)	(nc)	(nc)
	35	0.0006	16	0.56	2.2×10^{-9}	3.3×10^{-2}	0.55
Dichloromethane	25	0.0003	64	0.26	5.7×10^{-10}	2.3×10^{-1}	0.93
	27	0.0005	83	3.7	5.1×10^{-10}	5.3	19.5
	30	0.0007	43	0.037	(nc)	(nc)	(nc)
	30	0.0021	52	0.072	(nc)	(nc)	(nc)
	35	0.0027	43	0.19	1.2×10^{-9}	3.1×10^{-2}	0.28
	40	0.0021	29	0.27	1.6×10^{-9}	2.7×10^{-2}	0.31
Propylene Oxide	27	0.0005	89	0.0007	5.3×10^{-10}	1.3×10^{-4}	0.0005
	30	0.0005	115	0.0031	2.9×10^{-10}	6.7×10^{-2}	0.13
	30	0.0019	108	0.0084	(nc)	(nc)	(nc)
	35	0.0028	111	0.043	6.2×10^{-10}	4.6×10^{-2}	0.18

(continued)

TABLE 14. TEMPERATURE DEPENDENCE OF CHEMICAL PERMEATION THROUGH CHALLENGE 5200

Chemical	Temp. (°C)	MDR ($\mu g/cm^2$-min)	BT (min)	Reported rate ($\mu g/cm^2$-min)	D (cm^2/s)	S (g/cm^3)	Calculated steady-state rate ($\mu g/cm^2$-min)
Trichloroethylene	25	0.0011	49	0.19	3.6×10^{-10}	7.2×10^{-1}	1.9
	27	0.0011	72	0.0028	(nc)	(nc)	(nc)
	30	0.0011	34	0.14	(nc)	(nc)	(nc)
	35	0.0011	76	0.34	3.9×10^{-10}	1.2	3.4
	40	0.0011	81	0.48	4.8×10^{-10}	1.3×10^{-1}	0.47
Vinyl Acetate	25	0.0014	69	0.25	(nc)	(nc)	(nc)
	25	0.0003	73	38.0	4.7×10^{-10}	80.3	260.4
	25	0.0003	109	11.3	2.2×10^{-10}	1084.9	1733
	30	0.0021	101	0.089	(nc)	(nc)	(nc)
	35	0.0007	60	0.61	7.3×10^{-10}	1.7×10^{-1}	0.94
	40	0.0014	69	0.25	6.5×10^{-10}	4.9×10^{-2}	0.24

(nc) indicates no permeation-time curve was provided.

Figure 3. Temperature Dependence of Diffusion Coefficient Values

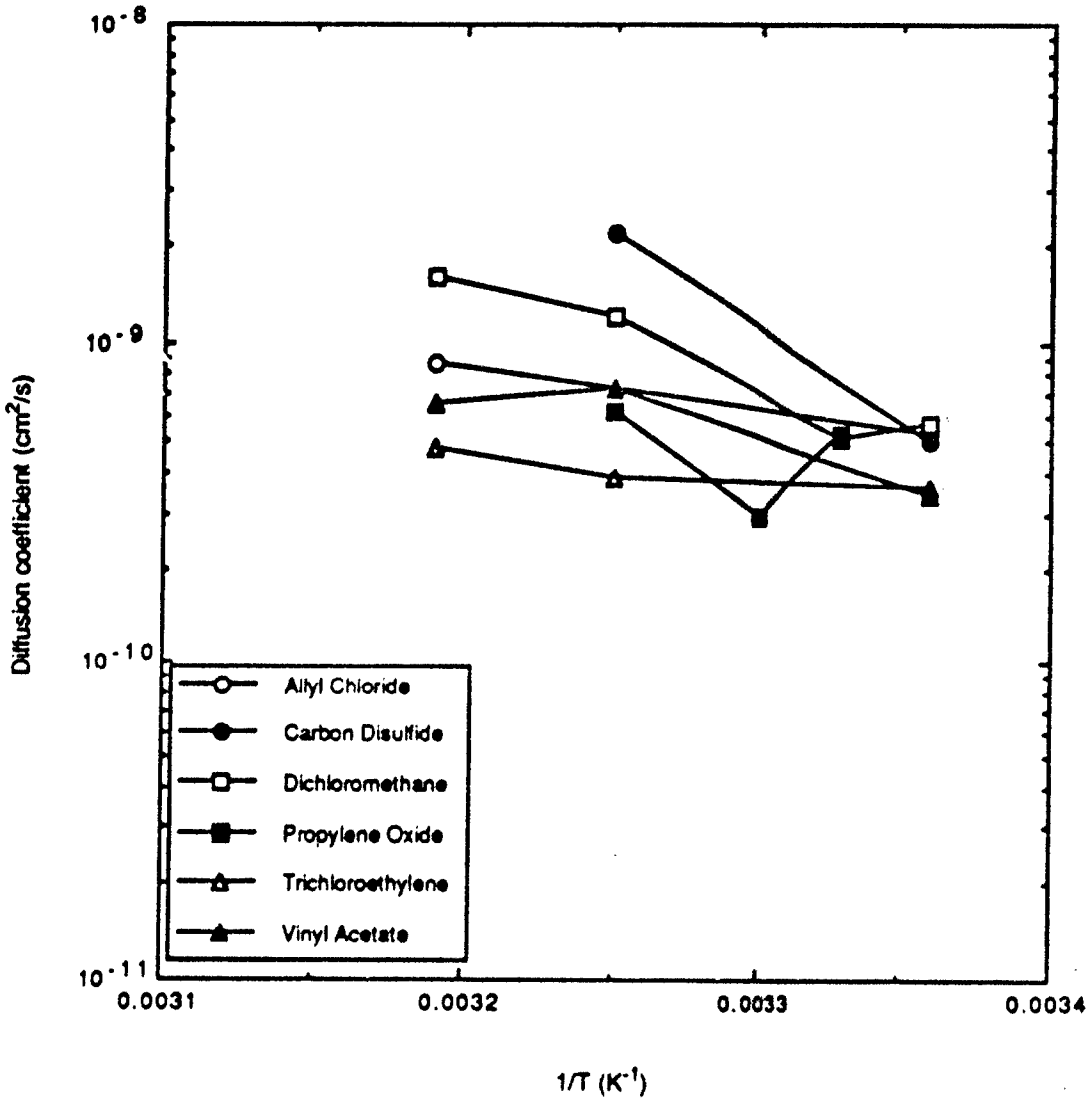


Figure 4. Temperature Dependence of Solubility Values

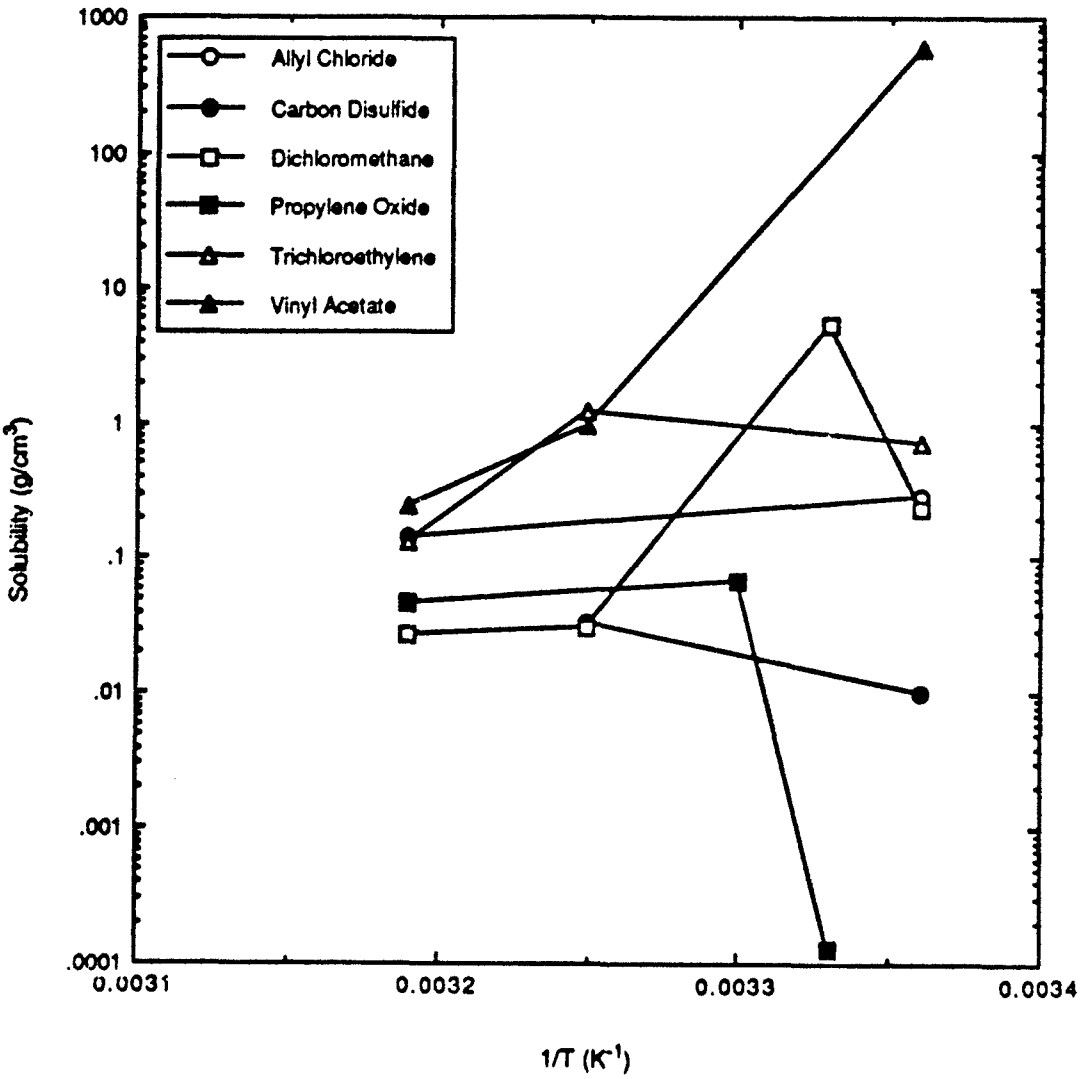
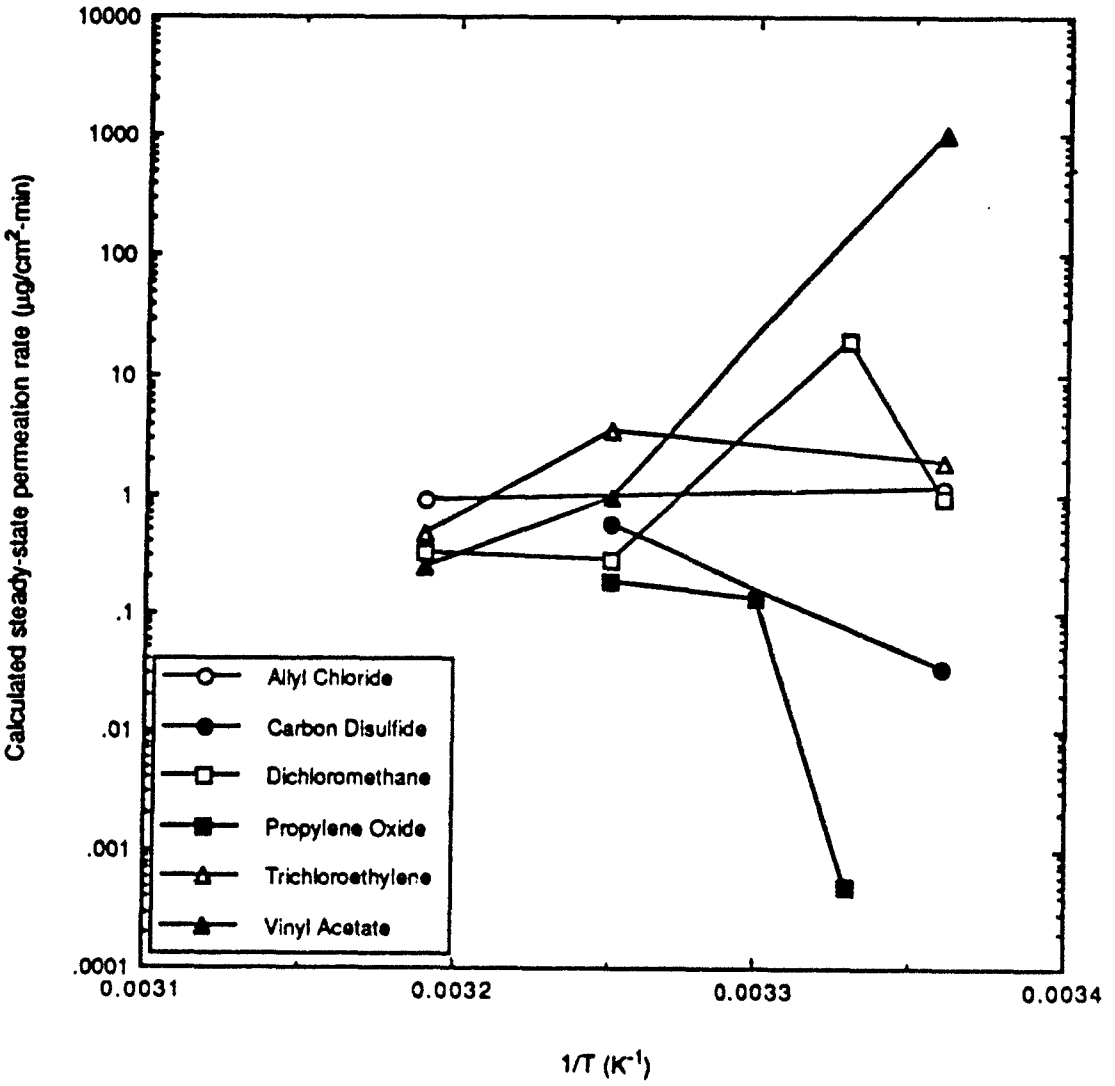


Figure 5. Temperature Dependence of Calculated Steady-State Permeation Rates



an Arrhenius relationship, such graphs would display a linear relationship between the logarithm of the parameter and the inverse temperature. For this data set, no consistent relationships are apparent, although the D values appear to show a small increase with temperature (i.e., decrease with increasing inverse temperature). Consequently, reliable conclusions regarding the temperature dependence of the barrier properties of the Challenge materials are not possible. The testing laboratory that generated the data could not provide insight into the cause for the inconsistencies. In order to achieve a better understanding of the temperature dependence, the tests should be repeated under better controlled test conditions.

4.1.3 Prediction of D and S Values

To extend the above analysis to develop a Fick's law-based predictive model for the data set at 25°C, one must develop techniques to predict D and S from basic properties of a chemical of interest. Several approaches to predicting these parameters have been developed although not for fluoropolymer-based materials [12,13]. Historically, the approaches have involved theoretical, empirical, and statistical correlations with properties of the chemical and polymer material and often depend on the type and size of database available.

Using the small set of values reported above, we briefly explored approaches to correlate/predict D and S. For D, we explored correlations with chemical properties that are representative of its size. We expected that fairly good correlations would be possible because, unlike the elastomers studied elsewhere [12,13], the fluoropolymer materials exhibit very little swelling and diffusion of the chemical through the polymer matrix might truly be controlled by molecular size considerations. Also, some preliminary work by the Coast Guard indicated that molecular size/minimum cross section of the permeant was an important variable in the permeation process [14]. Initial attempts at correlations are shown in Figure 6, in which the calculated values for D are plotted versus the permeant molecular weight, and in Figure 7, in which the D values are plotted versus permeant molar volume (liquid permeants only.) In both figures, however, the data show no definitive relation although there may be a trend of decreasing D with increasing molecular size.

Solubility prediction approaches generally involve correlations of properties that describe a chemical and material's interaction potential: solubility parameters, chemical interaction parameters, dipole moments, and state variables (EOS approaches). Others involve specific consideration of the chemical and polymer structure and use group-contribution approaches to describe the interactions of various structural groups and their contribution to chemical solubility in a polymer matrix. One such group-contribution approach, UNIFAP, has been applied with success to predict the solubilities of chemicals in rubbery polymers [12,15]. However, for fluoropolymer materials, the required group interaction parameters are only available for two chemical class types: hydrocarbons and fluorocarbons (saturated). Because permeation data were not available for these types of compounds, equilibrium solubility data from the literature were used to evaluate this technique [16]. Table 15 reports solubilities for several chemicals in polytetrafluoroethylene and predicted values using the UNIFAP technique. While there is good agreement for the hydrocarbon values, the predictions for the perfluorocarbon compounds greatly exceed the measured values.

Figure 6. Diffusion Coefficients versus Permeant Molecular Weight

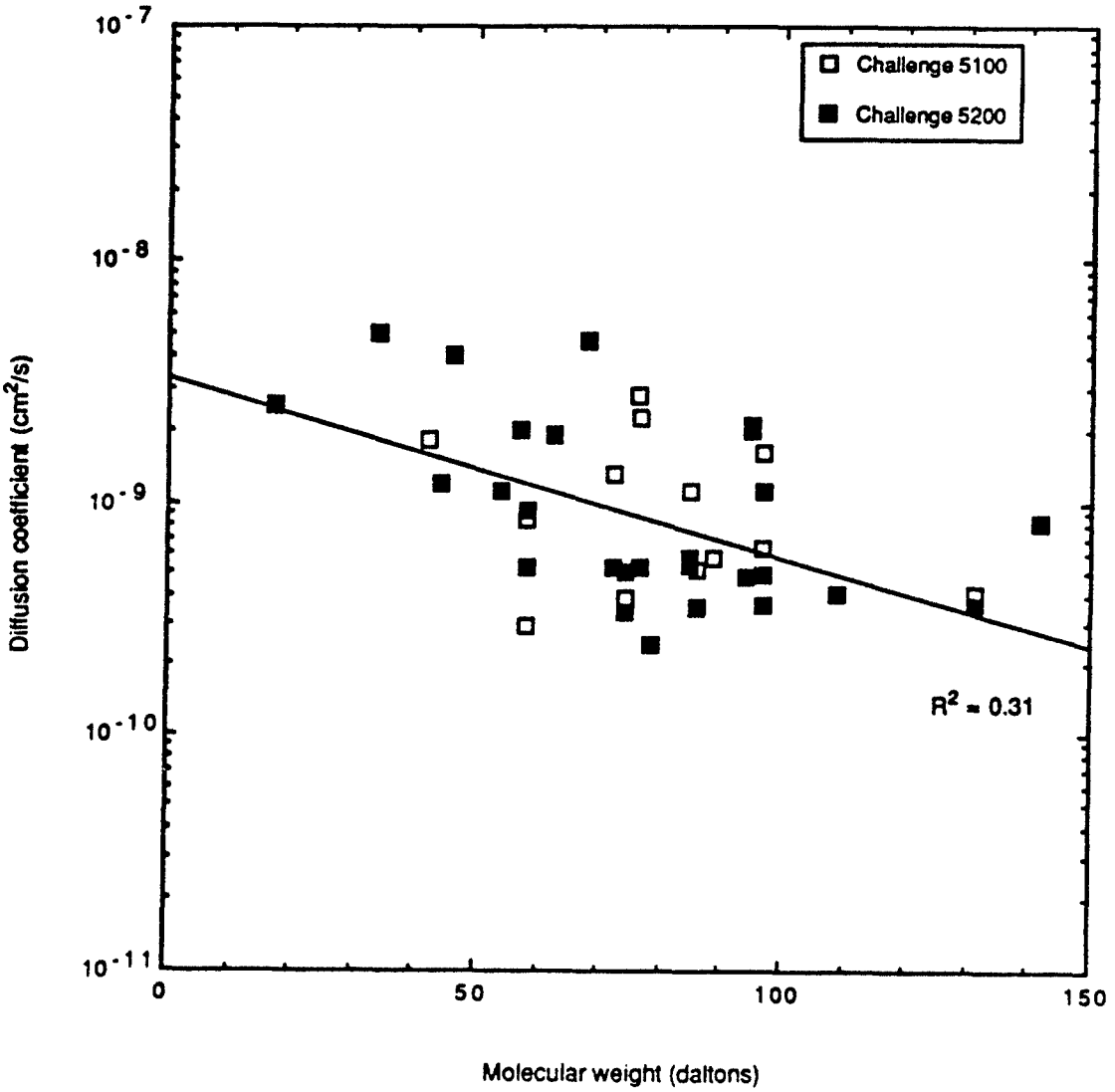


Figure 7. Diffusion Coefficients versus Permeant Molar Volume

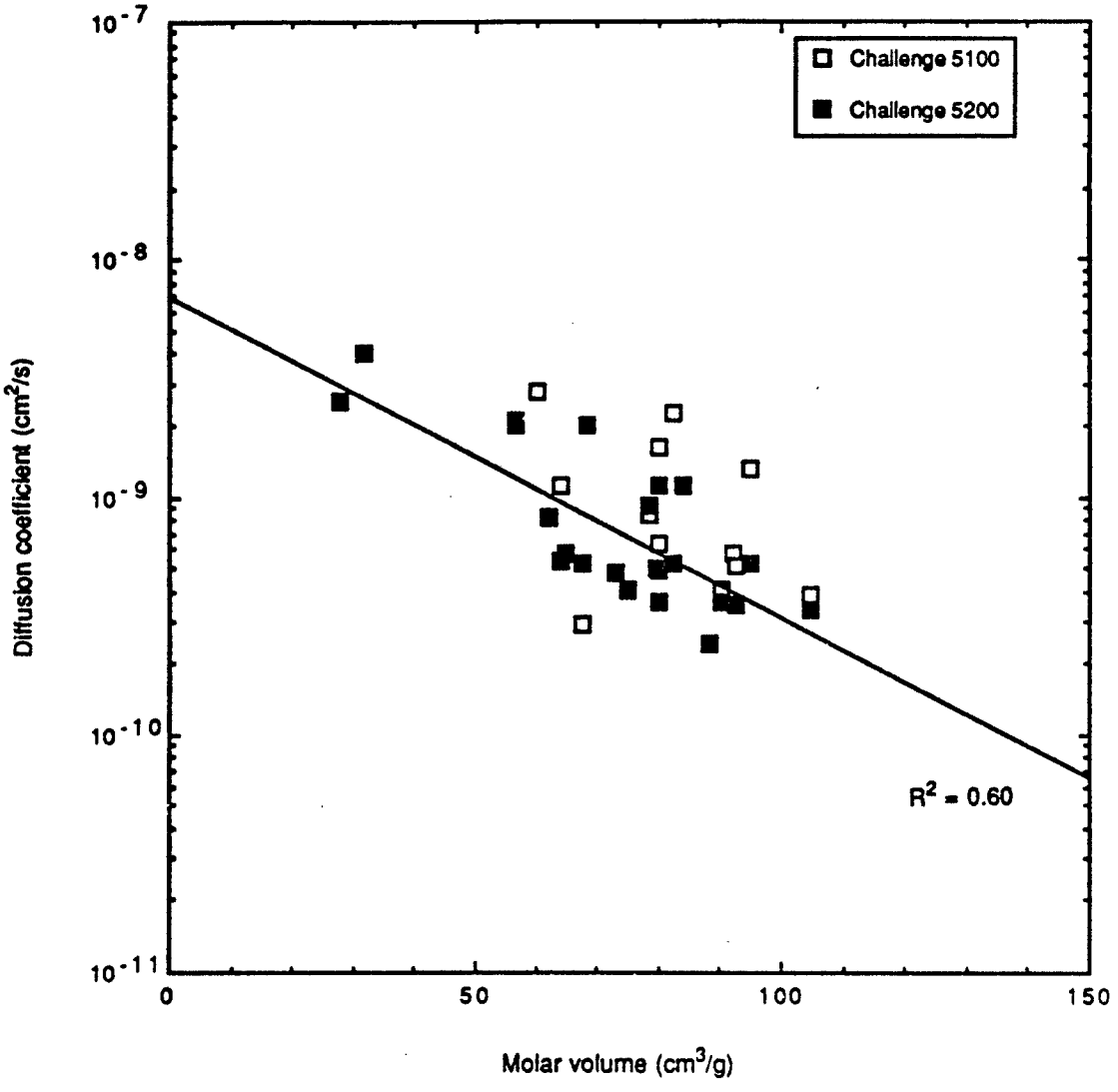


TABLE 15. SOLUBILITY PREDICTION FOR POLY(TETRAFLUOROETHYLENE) USING UNIFAP APPROACH

Chemical	Literature Data*		Predicted S (g/cm^3)
	Wt. gain (%)	Solubility (g/cm^3)	
HYDROCARBONS			
Cyclohexane	1.1	0.023	0.071
Heptane			0.029
Hexane	0.7	0.015	0.039
Octane	0.8	0.018	0.022
Pentane			0.048
PERFLUOROCARBONS			
Perfluorodimethylcyclohexane	10.1	0.23	
Perfluorocyclohexane			11.9
Perfluoroethane			9.4
Perfluoropropane			10.1
1,1,1-Trifluoroethane			5.7

* Results reported by Starkweather [16]. Equilibrium weight gains were converted to solubilities using poly(tetrafluoroethylene) density = 2.1 g/cm^3.

One other approach that was considered to predict S was using solubility parameters. Based on prior work by Hansen performed under contract to the Coast Guard [17-21], we evaluated the use of solubility parameters, both total and three-dimensional, to correlate the available S values. However, no correlations were identified. Other efforts regarding the use of solubility parameters are discussed in Section 4.2.

These efforts concluded our attempts to pursue a Fick's-law based predictive model. Because of our lack of success in predicting values for D and S, we abandoned our attempt to develop a quantitative model to predict permeation behavior as a function of time. Alternatively, we pursued empirical approaches to correlate the detection of permeation within 3 hours directly with properties descriptive of the permeating chemical: size, shape, and structure.

4.2 EMPIRICAL APPROACHES

4.2.1 Solubility Parameters

Solubility parameter approaches to predict chemical interactions have been pursued for several decades [22-24]. Much of this work was pioneered by Hansen, particularly regarding the application of three-dimensional solubility parameters [22,25]. In the past decade, solubility parameter correlations have been pursued to predict permeation of protective clothing materials and, since 1988, Hansen has been applying his three-dimensional solubility parameter approach to the Challenge material data set under contract to the Coast Guard. Although not pursued in our model development efforts, Hansen's findings are summarized briefly here because we applied solubility parameter considerations when selecting chemicals for our chemical mixture permeation tests as reported in Section 5.

Preliminary reports from 1988 describe efforts by Hansen to establish three-dimensional solubility parameter values for Challenge 5100 and to predict the Challenge 5100 data set [18-20]. The approach involved a combination of solubility parameter and molecular size considerations. A three-dimensional solubility parameter for Challenge 5100 was proposed and used to define the Relative Energy Difference (RED), a dimensionless parameter that describes the distance of a chemical from the center of a solubility parameter sphere divided by the sphere radius. The distance of the chemical from the sphere's center is calculated from the chemical's ($\delta_{d,c}$, $\delta_{p,c}$, $\delta_{h,c}$) and polymer's ($\delta_{d,p}$, $\delta_{p,p}$, $\delta_{h,p}$) three-dimensional solubility parameters as follows:

$$Distance = \sqrt{4(\delta_{d,c}-\delta_{d,p})^2+(\delta_{p,c}-\delta_{p,p})^2+(\delta_{h,c}-\delta_{h,p})^2} \qquad \text{Eq. (3)}$$

The RED is calculated using the following equation and a value for the radius established by Hansen:

RED=Distance/Radius Eq. (4)

The preliminary values reported by Hansen for Challenge 5100 were:

- $\delta_{d,p}$ = 17.1 $(J/cm^3)^{1/2}$
- $\delta_{p,p}$ = 8.1 $(J/cm^3)^{1/2}$
- $\delta_{h,p}$ = 1.3 $(J/cm^3)^{1/2}$
- Radius = 4.7

The predictive model proposed was that chemicals (or mixtures) with calculated RED values less than 1 (or 2 in some cases) and with molar volumes less than 103 cm^3/g would permeate Challenge 5100. Based on this preliminary finding, Hansen proposed several chemicals and chemical mixtures as priorities for testing by the Coast Guard. These tests were conducted through mid-1989. We also used this preliminary solubility parameter model when selecting the chemical mixtures for testing by Arthur D. Little in April 1989. The chemical mixture permeation test results and analysis are described in Section 5.

The preliminary model by Hansen demonstrated moderate success in predicting pure chemical permeation through the Challenge materials but little success in predicting chemical mixture permeation. Several of the Challenge 5100 permeation test results, however, could not be predicted with this model. Through analysis of the additional test results through mid-1989, Hansen proposed revised Challenge 5100 solubility parameter values, new Challenge 5200 solubility parameter values, and a refined model for permeation prediction [21]. These were:

- Challenge 5100
  - $\delta_{d,p}$ = 16.6 $(J/cm^3)^{1/2}$
  - $\delta_{p,p}$ = 5.4 $(J/cm^3)^{1/2}$
  - $\delta_{h,p}$ = 4.0 $(J/cm^3)^{1/2}$
  - Radius = 3.3
- Challenge 5200
  - $\delta_{d,p}$ = 16.6 $(J/cm^3)^{1/2}$
  - $\delta_{p,p}$ = 6.0 $(J/cm^3)^{1/2}$
  - $\delta_{h,p}$ = 4.8 $(J/cm^3)^{1/2}$
  - Radius = 3.7
- Predictive model
  - Monomers: permeation will occur if RED < 1 and molar volume < 100 cm^3/g
  - Other chemicals: permeation will occur if RED < 1 and molar volume < 75 cm^3/g

The revised solubility parameter values and model provided a better fit to the data set although several outlier predictions remain. As noted in Section 3, some outliers may be the

result of discrepancies within the data set itself. The prediction of chemical mixture behavior is still not successful using the revised model.

In summary, the solubility parameter approach has demonstrated success in describing the present data set in terms of whether individual chemicals will permeate the Challenge materials within 3 hours. The empirical model can be used to predict whether permeation will occur for untested chemicals if a value for the three-dimensional solubility parameter is available for the chemical of interest. Another important finding by Hansen was that molecular size, in addition to solubility parameter, was a critical variable controlling the permeation behavior.

4.2.2 Molecular Modeling

Molecular modeling was pursued by us as an aid to developing an empirical model to predict permeation of the Challenge fabrics. Our specific goal was to explore molecular size and shape considerations reported earlier by Bentz et. al. [14] as important parameters. Molecular modelling software (Alchemy®, Tripos Associates) was used to examine the role of molecular size. Models were drawn of both permeating and non-permeating chemicals. Two aspects of size were considered: physical size (cross-sectional area and total volume), and molecular weight. Physical size was found to be more important than molecular weight in predicting permeation behavior.

With one exception (methyl acrylate), no chemical tested having greater than five non-hydrogen atoms permeates either fabric under the test conditions. This indicates that the molecular volume of five non-hydrogen atoms appears to be too large to enable permeation through the materials.

In general, chemicals tested with three or less non-hydrogen atoms permeate the materials under the test conditions. Only very polar compounds of this size such as inorganic acids and ionic compounds were not observed to permeate.

For chemicals of intermediate size (i.e., four or five non-hydrogen atoms), the electronic surface appears to be a more important determinant of permeation then absolute molecular size. Two molecules of identical size can have very different permeation characteristics. Neither very non-polar (butane) nor very polar (acetic acid) molecules permeate the materials. A necessary requirement for permeation appears to be the presence of functional groups of intermediate polarizability. These functional groups include carbon-carbon double bonds and halogen atoms. These groups have approximately the same degree of polarizability as the functional groups of the fluoropolymer barrier films in the Challenge fabrics. This observation is consistent with the identified solution-diffusion mechanism of permeation. Materials of like polarizability are most likely to be mutually soluble.

Attempts were made to correlate these observations with a physical property or properties of the chemicals, however, no correlation that adequately predicted the entire data set was identified. We found that the simplest and most accurate approach to predict the permeation data set was an empirical model that considered molecular structure, addressing both size and the presence of certain functional groups.

4.3 EMPIRICAL MODEL TO PREDICT PURE CHEMICAL PERMEATION

Based on the above observations, a series of rules was developed to aid in predicting which compounds might permeate the Challenge materials. The set of rules predict whether permeation of Challenge 5100 or Challenge 5200 will occur within 3 hours at 25°C at a detection sensitivity of 0.05 $\mu g/cm^2$-min. This detection sensitivity was selected because it approximates the average detection sensitivity reported in the permeation test program. However, as noted in Section 3, there was a wide range in the detection sensitivities used in the testing which complicated direct comparison of many of the results provided for this model development effort.

The initial set of rules, proposed in late-1988, was able to correctly predict the permeation behavior of 94% of the chemicals tested by that time. Based on these rules, priority chemicals were identified for future testing to evaluate the prediction accuracy of the rule set. These tests (and others) were conducted by the Coast Guard through 1989 and the results were compared to the predictions of the initial rule set. The rule set predicted correctly for 76% of the compounds. Many of these compounds were deliberately selected to test the limits of the rule set and, thus, aided in refining the rules.

On the basis of the expanded data set, the rules were modified slightly. The revised set correctly predicts the permeation behavior for 88 to 93% of the chemicals in the full data set. The final set of rules to predict permeation of Challenge 5100 or Challenge 5200 within 3 hours at 25°C and a detection sensitivity of 0.05 $\mu g/cm^2$-min is as follows:

A. Compounds Containing Three (3) or Less Non-Hydrogen Atoms:

1. Acidic compounds (pKa < 3) will not permeate (e.g., inorganic acids such as hydrochloric).

2. Ionic compounds will not permeate.

3. All other compounds will permeate.

B. Compounds Containing Four (4) or Five (5) Non-Hydrogen Atoms:

1. If the compound does not contain either a carbon-carbon double bond or a halogen atom, it will not permeate.

2. Inorganic compounds will not permeate.

3. If the compound contains four (4) or more saturated (tetrasubstituted) carbon atoms, it will not permeate.

4. If the compound contains four (4) or more halogen atoms, it will not permeate.

5. If the compound has two (2) or more non-halogen substituents on a carbon-carbon double bond, it will not permeate.

6. If the compound contains any of the following polar functional groups, it will not permeate.

- Alcohol
- Aldehyde
- Amine
- Carboxylic acid
- Ketone
- Nitro
- Nitroso
- Any sulfur containing group

7. All other compounds will permeate.

C. Compounds Containing Six (6) or Greater Non-Hydrogen Atoms:

1. The compound will not permeate.

This revised rule set was used to predict permeation for the full data set to evaluate its accuracy. In total, predictions were made for 262 chemicals. The permeation data reported for nine of these 262 chemicals, however, indicated conflicting results so that determination of a "correct" prediction could not be made. These chemicals are listed in Table 16 and were not considered in judging the accuracy of the rule set. Of the remaining 253 chemicals, incorrect predictions were found for 30 chemicals (12%). However, several of these incorrect predictions can be resolved when the MDR values reported for the various tests are considered.

For example, Table 17 reports the 10 chemicals for which the model predicts no permeation should occur (within three hours at 25°C at an MDR of 0.05 $\mu g/cm^2$-min) but the test results indicate that permeation was observed. For nine of these chemicals, however, the reported MDRs were at least one order of magnitude lower than the target MDR for the model prediction. Table 18 identifies the remaining 20 chemicals for which the model predicts permeation but test results indicate that no permeation was observed. For four of these chemicals, as noted in the table, the reported MDRs were higher than the target MDR for the model, so these tests were less sensitive than most considered in the model development. If these 13 chemicals with MDR considerations are not counted, the chemicals with incorrect predictions drop to 17 of 253 (7%).

TABLE 16. PERMEATION MODEL PREDICTIONS FOR CHEMICALS WITH CONFLICTING PERMEATION TEST RESULTS

Chemical	Model*	Data**	MDR ($\mu g/cm^2$-min)	Comments
Acetone	N	Y/N	0.00004 0.040	Permeation only at 27°C or higher
Ammonia gas	Y	Y/N	0.0005 0.001	
Ammonium hydroxide	Y	Y/N	0.0071 0.057	
Freon 12	N	Y/N	0.0098 0.34	Permeation detected in only 1 of 6 replicates
Ethyl ether	N	Y/N	0.0006 0.0078	Permeation only at low MDR and/or 27°C
Methyl acrylate	N	Y/N	0.0083 0.49	Permeation not detected at lower MDR
Tetrachloroethylene	N	Y/N	0.0001 0.015	Permeation detected in 1 of 4 replicates
Trimethylamine	N	Y/N	0.0007 0.007	Permeation not detected at lower MDR in repeat test
Vinylidene fluoride	Y	Y/N	0.0021 0.036	Permeation detected at lower MDR in repeat test

* Model prediction as to whether permeation will occur within 180 minutes at 25°C at a detection limit of 0.05 $\mu g/cm^2$-min: Y = Yes, N = No.

** Permeation test results indicating whether permeation was detected: Y = Yes, N = No, Y/N = Multiple or replicate tests indicate that permeation both was and was not detected.

TABLE 17. CHEMICALS FOR WHICH THE MODEL PREDICTS PERMEATION BUT TESTS INDICATE NO PERMEATION

Chemical	Model*	Data**	MDR ($\mu g/cm^2$-min)	Comments
Acetaldehyde	Y	N	Not reported	
Acetonitrile	Y	N	0.033;0.066	
Allyl bromide	Y	N	0.0010	
Bromine	Y	N	0.068	High MDR
Cyanogen bromide	Y	N	0.086	High MDR
Cyanogen chloride	Y	N	0.025	
Dibromomethane	Y	N	0.0070;0.0042	
1,3-Dichloropropene	Y	N	0.015	
Ethane	Y	N	0.024	
Ethanol	Y	N	0.11	High MDR
Ethylamine	Y	N	0.027	
Ethyleneimine	Y	N	0.00040	
Ethylene sulfide	Y	N	0.015	
Ethylene	Y	N	0.0020	
Formaldehyde solution	Y	N	Not reported	
Hydrazine hydrate	Y	N	0.023	Prediction based on hydrazine
Hydrogen peroxide	Y	N	0.017	
Methanol	Y	N	0.11	High MDR
Methylamine	Y	N	0.0050	
Propane	Y	N	0.00040	

* Model prediction as to whether permeation will occur within 180 minutes at 25°C at a detection limit of 0.05 $\mu g/cm^2$-min; Y = Yes, N = No.

** Permeation test results indicating whether permeation was detected; Y = Yes, N = No.

TABLE 18. CHEMICALS FOR WHICH THE MODEL PREDICTS NO PERMEATION BUT TESTS INDICATE PERMEATION

Chemical	Model*	Data**	MDR ($\mu g/cm^2$-min)	Comments
Acrolein	N	Y	0.0054	Low MDR
2-Butene	N	Y	0.0018	27°C, low MDR
Cyanogen	N	Y	0.021	
Isoprene	N	Y	0.00050	Low MDR
Methyl acetate	N	Y	0.0012	Low MDR
Methyl chloroformate	N	Y	0.0038	Low MDR
Methyl isocyanate	N	Y	0.00050	Low MDR
Nitrogen tetroxide	N	Y	0.0059	Low MDR
Phosgene	N	Y	0.5 ppm	27°C, Low MDR
Propylene oxide	N	Y	0.0005;0.008	Low MDR

* Model prediction as to whether permeation will occur within 180 minutes at 25°C at a detection limit of 0.05 $\mu g/cm^2$-min; Y = Yes, N = No.

** Permeation test results indicating whether permeation was detected; Y = Yes, N = No, Y/N = Multiple or replicate tests indicate that permeation both was and was not detected.

This prediction accuracy of 88 to 93% is quite good considering the lack of consistency in portions of the data set, particularly regarding the MDRs. Possibly, some of the chemicals for which incorrect predictions were found should be retested.

These rules were organized into a decision tree in the form of a series of questions with yes or no answers regarding the chemical's structure that leads to a Yes/No prediction of permeation. One benefit of this approach is that no information other than the structure of a chemical is required to make a prediction. In most applications, information on a chemical's structure can be readily obtained. The rules/decision tree questions are illustrated in flowcharts in Appendix F. The rules/decision tree were also computerized as described in Section 6 to simplify the use of this empirical model by Coast Guard field personnel.

SECTION 5

DEVELOPMENT OF MODEL TO PREDICT CHEMICAL MIXTURE PERMEATION

5.1 ANALYSIS OF CHEMICAL MIXTURE DATA

5.1.1 TRI Mixture Permeation Test Results

The results of the permeation tests with 29 chemical mixtures conducted by TRI are summarized in Appendix C. The mixtures span a range of chemical classes and include both two- and three-component mixtures. Also, the mixtures include combinations of chemicals in which only one component was known to permeate as well as those in which both (or all three) components were known to permeate. Only the breakthrough times were reported for these tests, no permeation rates were measured. Although individual MDRs and breakthrough times are reported for each mixture component in most of the Challenge 5100 tests, the results for the Challenge 5200 tests were reported only as generic breakthrough times without identifying the permeating species. These results are noted in Appendix C.

The results are summarized and compared in Table 19 for both Challenge 5100 and Challenge 5200. The table combines and reports the results alphabetically by mixture component. Each chemical tested in a mixture is listed separately in the table. Thus, for each chemical, the results of all mixture tests with that chemical are listed as well as any pure chemical test results. In all cases, the results for the pure chemical are listed in the first row (or rows). Subsequent rows list the results of all mixture tests involving that chemical. For example, Table 19 begins with acetone and reports the average results of the pure chemical tested against Challenge 5100 and Challenge 5200. The table then lists the results of all mixture permeation tests in which acetone was a component. In this case, there were eight such tests performed. For these tests, the table lists the reported breakthrough times for each mixture component. Because of this format, the results of each mixture test are reported multiple times, once for each component in the mixture in alphabetical order. This format was selected because it simplifies comparison of the results and facilitates comparison with the pure chemical results.

Review of this table indicates that, in essentially all cases, the permeation of the chemicals from the various chemical mixtures can be predicted directly from the behavior when tested as a pure chemical. If a mixture component was found to permeate when tested as a pure chemical, it was found to permeate from the mixture and at approximately the same or slightly longer breakthrough time. If a mixture component did not permeate when tested as a pure chemical, it also was not found to permeate from a mixture. Two exceptions to this rule exist: acetonitrile and nitromethane. In the case of acetonitrile, permeation was not detected when tested as a pure chemical at MDLs of 1.0 and 2.0 ppm. In the mixture tests, acetonitrile permeation was detected but at an MDL of 0.02 ppm. In the other case, the MDLs for nitromethane were similar in the various tests, however, permeation was detected in one pure chemical test with Challenge 5200 but not in the test with Challenge 5100 or the

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

Mixture					Component #1		Component #2		Component #3	
Component #1	Component #2	Component #3	Material		MDL (ppm)	BT (min)	MDL	BT	MDL (ppm)	BT (min)
Acetone	--	--	5100		1.20	> 210				
	--	--	5200		1.00	> 180				
	Chlorobenzene	--	5200	•	0.10	> 180	0.10	> 180		
	1,2-Dichloroethane	--	5200	•	0.82	> 180	0.82	> 180		
	Epichlorohydrin	--	5200	•	0.14	> 180	0.14	> 180		
	Nitrobenzene	--	5200	•	0.02	> 180	0.02	> 180		
	Toluene	--	5200	•	0.01	> 180	0.01	> 180		
	Toluene	Methyl Ethyl Ketone	5200	•	0.01	> 180	0.01	> 180	0.01	> 180
	Toluene	Nitrobenzene	5200	•	0.02	> 180	0.02	> 180	0.02	> 180
	Vinyl Acetate	--	5100		0.01	> 180	0.01	120		
Acetonitrile	--	--	5100		1.00	> 180				
	--	--	5200		2.00	> 180				
	Chlorobenzene	--	5100		0.02	93	0.01	> 180		
	1,2-Dichloroethane	--	5100		0.02	85, >180	0.01	> 180		
	Nitrobenzene	--	5100		0.02	80	0.01	> 180		
	Chlorobenzene	Nitrobenzene	5100		0.02	80	0.01	> 180	0.01	> 180
Acrylonitrile	--	--	5100		0.46	65				
	Trichloroethylene	--	5100		0.01	120-140	0.01	60-80		
Benzene	--	--	5100		0.05	> 192				
	Dimethyl Sulfoxide	--	5200	•	0.01	> 180	0.01	> 180		
	Dimethyl Sulfoxide	1,2-Dichloroethane	5200	•	0.01	> 180	0.01	> 180	0.01	> 180
Carbon Disulfide	--	--	5100		0.10	20				
	--	--	5200		0.01	20				
	Dichloromethane	(75%) --	5100	••	0.02	12	0.02	12		

(Continued)

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

Mixture					Component #1		Component #2		Component #3	
Component #1	Component #2	Component #3	Material		MDL (ppm)	BT (min)	MDL (ppm)	BT (min)	MDL (ppm)	BT (min)
Carbon Disulfide (cont.)	Dichloromethane	(50%) --	5100	**	0.55	17	0.55	17		
	Dichloromethane	(25%) --	5100	**	0.03	16	0.03	16		
	Dimethylformamide	--	5100		0.01	12	0.01	> 180		
Chlorobenzene	--	--	5100		0.20	> 180				
	Acetone	--	5200	*	0.01	> 180	0.01	> 180		
	Acetonitrile	--	5100		0.01	> 180	0.02	93		
	Acetonitrile	Nitrobenzene	5100		0.01	> 180	0.02	80	0.01	> 180
	Dichloromethane	--	5100		0.01	> 180	0.02	81		
Chloroform	--	--	5100		0.19	> 216				
	Dimethylformamide	--	5200	*	0.07	> 180	0.07	> 180		
	Dimethyl Sulfoxide	--	5200	*	0.01	> 180	0.01	> 180		
	Nitromethane	--	5200	*	0.55	> 180	0.55	> 180		
1,2-Dichloroethane	--	--	5100		0.09	> 342				
	Acetone	--	5200	*	0.82	> 180	0.82	> 180		
	Acetonitrile	--	5100		0.01	> 180	0.02	85, > 180		
	Benzene	Dimethyl Sulfoxide	5200	*	0.01	> 180	0.01	> 180	0.01	> 180
Dichloromethane	--	--	5100		0.27	51				
	--	--	5200		0.01	83				
	Carbon Disulfide	(75%) --	5100	**	0.03	16	0.03	16		
	Carbon Disulfide	(50%) --	5100	**	0.55	17	0.55	17		
	Carbon Disulfide	(25%) --	5100	**	0.02	12	0.02	12		
	Chlorobenzene	--	5100		0.02	81	0.01	> 180		
	Nitrobenzene	--	5100		0.02	56	0.01	> 180		
	Trichloroethylene	(75%) --	5100	**	0.06	47	0.06	47		

(Continued)

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

Mixture					Component #1		Component #2		Component #3	
Component #1	Component #2	Component #3	Material		MDL (ppm)	BT (min)	MDL (ppm)	BT (min)	MDL (ppm)	BT (min)
Dichloromethane (cont.)	Trichloroethylene	(50%) --	5100	**	0.03	68	0.03	68		
	Trichloroethylene	(25%) --	5100	**	0.05	105	0.05	105		
Dimethylformamide	--	--	5100		nd	> 192				
	Carbon Disulfide	--	5100		0.01	> 180	0.01	12		
	Chloroform	--	5200	*	0.07	> 180	0.07	> 180		
Dimethyl Sulfoxide	--	--	5200		0.01	> 180				
	Benzene	--	5200	*	0.01	> 180	0.01	> 180		
	Benzene	1,2-Dichloroethane	5200	*	0.01	> 180	0.01	> 180	0.01	> 180
	Chloroform	--	5200	*	0.01	> 180	0.01	> 180		
Epichlorohydrin	--	--	5100		0.75	> 180				
	Acetone	--	5200	*	0.14	> 180	0.14	> 180		
Methyl Ethyl Ketone	--	--	5100		0.65	> 180				
	Acetone	Toluene	5200	*	0.01	> 180	0.01	> 180	0.01	> 180
	2-Nitropropane	Toluene	5200	*	0.82	> 180	0.82	> 180	0.82	> 180
Nitrobenzene	--	--	5100		0.08	> 180				
	Acetone	--	5200	*	0.02	> 180	0.02	> 180		
	Acetone	Toluene	5200	*	0.02	> 180	0.02	> 180	0.02	> 180
	Acetonitrile	--	5100		0.01	> 180	0.02	80		
	Acetonitrile	Chlorobenzene	5100		0.01	> 180	0.02	80	0.01	> 180
	Dichloromethane	--	5100		0.01	> 180	0.02	56		
	Toluene	--	5200	*	0.01	> 180	0.01	> 180		
Nitromethane	--	--	5100		0.26	> 180				

(Continued)

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

Mixture					Component #1		Component #2		Component #3	
Component #1	Component #2	Component #3	Material		MDL (ppm)	BT (min)	MDL (ppm)	BT (min)	MDL (ppm)	BT (min)
Nitromethane (cont.)	--	--	5200		0.73	168				
	--	--	5200		0.70	> 180				
	Chloroform	--	5200	*	0.55	> 180	0.55	> 180		
2-Nitropropane	--	--	5100		0.59	> 180				
	Methyl Ethyl Ketone	Toluene	5200	*	0.82	> 180	0.82	> 180	0.82	> 180
Toluene	--	--	5100		0.06	> 180				
	Acetone	--	5200	*	0.01	> 180	0.01	> 180		
	Acetone	Methyl Ethyl Ketone	5200	*	0.01	> 180	0.01	> 180	0.01	> 180
	Acetone	Nitrobenzene	5200	*	0.02	> 180	0.02	> 180	0.02	> 180
	Methyl Ethyl Ketone	2-Nitropropane	5200	*	0.82	> 180	0.82	> 180	0.82	> 180
	Nitrobenzene	--	5200	*	0.01	> 180	0.01	> 180		
Trichloroethylene	--	--	5100		0.07	143				
	--	--	5200		0.01	61				
	Acrylonitrile	--	5100		0.01	60-80	0.01	120-140		
	Dichloromethane	(75%) --	5100	**	0.05	105	0.05	105		
	Dichloromethane	(50%) --	5100	**	0.03	68	0.03	68		
	Dichloromethane	(25%) --	5100	**	0.06	47	0.06	47		
Vinyl Acetate	--	--	5100		0.21	106				
	--	--	5200		0.01	84				
	Acetone	--	5100		0.01	120	0.01	> 180		

* Reported MDL values did not indicate whether they were for specific mixture components or generic values for the mixture.

** Reported MDL values are generic values for the mixture. The breakthrough times report the time at which some component was detected but the specific component was not identified.

repeat test with Challenge 5200. No permeation was detected prior to concluding the one mixture test at 180 minutes. In the pure chemical test in which permeation was detected, the breakthrough time, 168 minutes, approaches the test termination time so the apparent discrepancy is not surprising.

Because no synergistic effects were observed, the results could be interpreted as further support of a solution-diffusion mechanism with the mixture components behaving independently. This is usually not the case for elastomeric protective clothing materials, in which swelling and chemical synergies produce unexpected and non-ideal behavior [26,27]. To further explore the mixture permeation behavior, supplementary tests were conducted by Arthur D. Little as described below.

5.1.2 Supplementary Tests to Explore Behavior as Function of Time

We conducted a series of tests that involved two- and three-component mixtures of three chemicals: carbon disulfide, vinyl acetate, and ethanol. Mixtures of various combinations and concentrations were tested to explore the effect of concentration on the permeation behavior. Permeation rates as a function of time were measured. Pure chemical tests were also conducted for baseline values. Carbon disulfide was selected because of its fast breakthrough and high permeation rate. Vinyl acetate was selected for its intermediate permeation properties. Ethanol was selected because it did not permeate (within three hours.) These chemicals were also selected to test the solubility parameter approach proposed by Hansen to predict permeation behavior. Table 20 identifies the mixtures that were tested and lists the RED values calculated for these chemicals. At the time the mixtures were selected only the preliminary solubility parameter values for Challenge 5100 were available and thus were used. Because both carbon disulfide and vinyl acetate were known to permeate, mixtures at several concentrations of these two compounds were selected to study the effect of concentration. The remaining mixtures involved ethanol, a chemical not detected to permeate, in an attempt to produce mixtures that would increase ethanol permeation or "carry" ethanol through the material.

The detailed results of these tests are reported in Appendix D. A summary of the results is provided in Table 21. In general, the breakthrough times for the mixture components were relatively constant for that component in each mixture compared to the value measured as a pure chemical. Note that in these tests, ethanol was detected to permeate but at very long times, almost 6 hours. The permeation rates of the mixture components, however, were often reduced relative to those measured as pure compounds in proportion to their concentration in the mixture (i.e., as the concentration was decreased, the steady-state permeation rate decreased although not in a direct proportion). The behavior of the carbon disulfide/vinyl acetate mixture behavior as a function of time and concentration is shown in Figures 8 and 9. Figure 8 illustrates the permeation of carbon disulfide and Figure 9 illustrates the permeation of vinyl acetate at the various mixture concentrations. The permeation of the carbon disulfide had the smallest concentration effect (i.e., reduction in permeation rate as the concentration was reduced) and, for mixtures with ethanol, the carbon disulfide permeation rates measured were similar to that for the pure compound.

TABLE 20. SUPPLEMENTARY CHEMICAL MIXTURE TESTED AND HANSEN SOLUBILITY PARAMETERS

Test #	Component(s)	Comp. (vol. %)	Solubility Parameters $(J/cm^3)^{1/2}$			RED*	
			Disp.	Polar	Hyd.	C-5100-p	C-5200
1	Carbon Disulfide	100	19.9	5.8	0.6	1.3	2.1
2	Vinyl Acetate	100	16.0	7.2	5.9	1.1	0.5
3	Ethanol	100	15.8	8.8	19.4	3.9	4.0
4	Carbon Disulfide/Vinyl Acetate	90/10	19.5	5.9	1.1	1.1	1.9
5	Carbon Disulfide/Vinyl Acetate	50/50	18.0	6.5	3.3	0.6	0.9
6	Carbon Disulfide/Vinyl Acetate	10/90	16.4	7.1	5.4	0.9	0.3
7	Carbon Disulfide/Ethanol	50/50	17.9	7.3	10.0	1.9	1.6
8	Vinyl Acetate/Ethanol	50/50	15.9	8.0	12.7	2.5	2.2
9	Carbon Disulfide/Vinyl Acetate/Ethanol	45/45/10	17.7	6.7	4.9	0.9	0.6
10	Carbon Disulfide/Vinyl Acetate/Ethanol	25/25/50	16.9	7.7	11.3	2.1	1.8

* RED calculated using Eq. (4) and solubility parameter values reported by Hansen for Challenge materials: C-5100-p uses preliminary values reported for Challenge 5100 in 1988, C-5200 uses values reported for Challenge 5200 in 1989.

TABLE 21. CHEMICAL MIXTURE PERMEATION RESULTS FOR CHALLENGE 5200
Temperature = 23-26°C

Chemical Challenge	Average* breakthrough (min)**			Average* steady-state rate (µg/cm²-min)		
	Carbon Disulfide	Vinyl Acetate	Ethanol	Carbon Disulfide	Vinyl Acetate	Ethanol
Carbon Disulfide	46	--	--	0.58	--	--
Vinyl Acetate	--	37	--	--	0.060	--
Ethanol	--	--	277	--	--	0.0037
Carbon Disulfide/Vinyl Acetate (90/10) +	43	124	--	0.52	0.018	--
Carbon Disulfide/Vinyl Acetate (50/50)	57	87	--	0.46	0.042	--
Carbon Disulfide/Vinyl Acetate (10/90)	75	61	--	0.30	0.058	--
Carbon Disulfide/Ethanol (50/50)	37	--	349	0.74	--	NR++
Vinyl Acetate/Ethanol (50/50)	--	71	>450	--	0.025	ND++
Carbon Disulfide/Vinyl Acetate/Ethanol (45/45/10)	41	71	393	0.65	0.052	NR
Carbon Disulfide/Vinyl Acetate/Ethanol (25/25/50)	48	96	444	0.52	0.035	NR

* Average of three replicate tests

** Breakthrough was detected at the following minimum detectable permeation rates: Carbon Disulfide: 0.060 µg/cm²-min; Vinyl Acetate: 0.0020 µg/cm²-min; Ethanol: 0.0020 µg/cm²-min.

\+ Percents by volume

++ NR: Steady-state not reached, ND: None detected

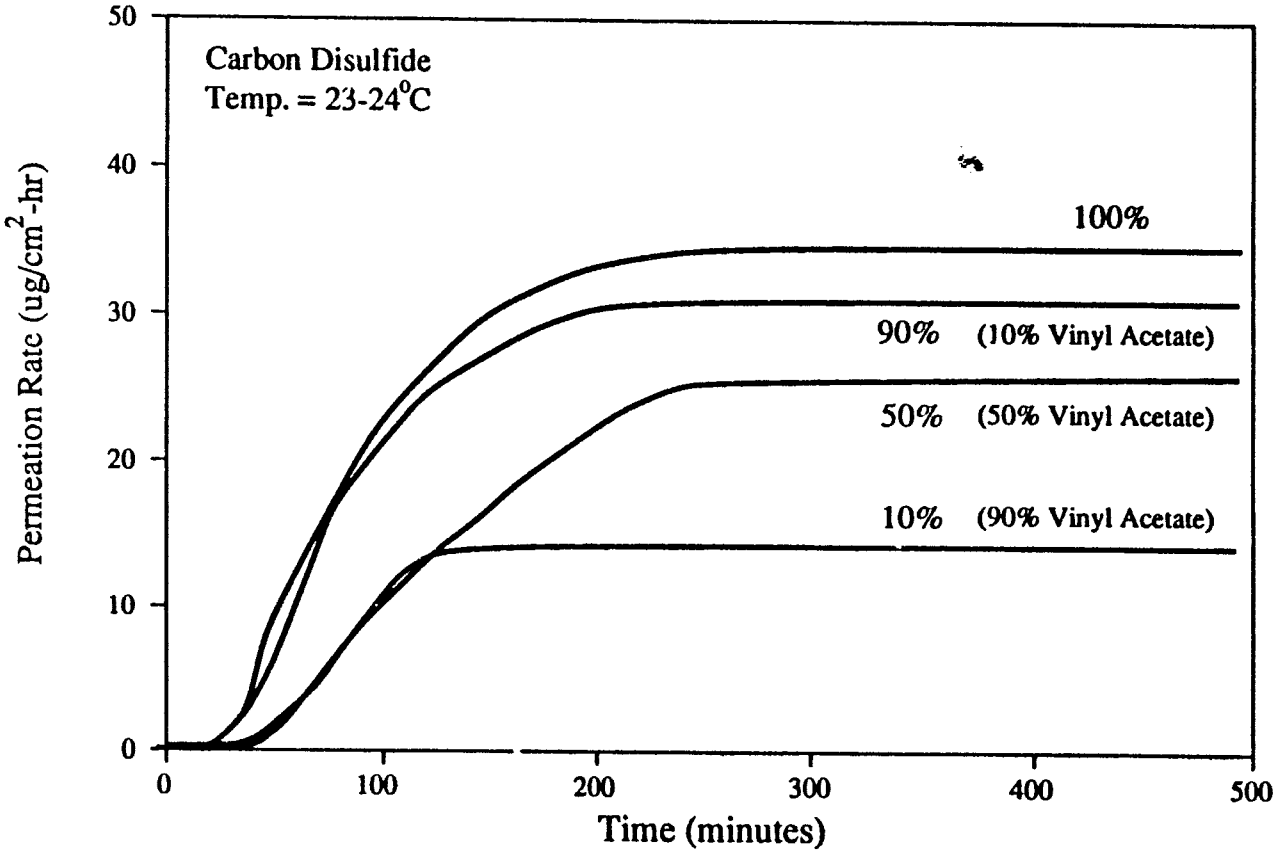


Figure 8. Permeation of carbon disulfide from carbon disulfide/vinyl acetate mixtures through Challenge 5200

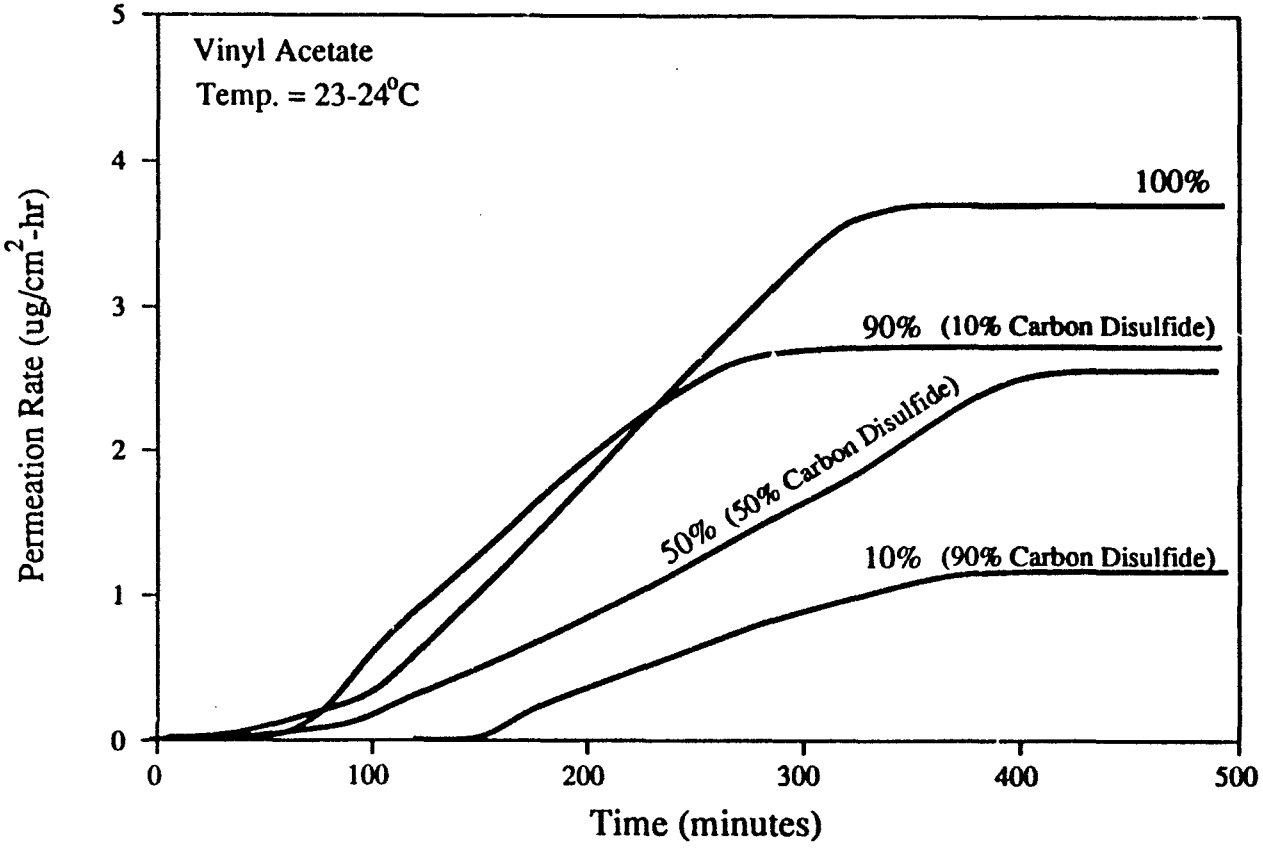


Figure 9. Permeation of vinyl acetate from carbon disulfide/vinyl acetate mixtures through Challenge 5200

5.2 EMPIRICAL MODEL TO PREDICT CHEMICAL MIXTURE PERMEATION

Although the supporting data base is small, a general rule is proposed to predict chemical mixture permeation through the Challenge materials, again at 25°C and within three hours at a representative detection sensitivity of 0.05 $\mu g/cm^2$-min:

- If the chemical permeates in pure form, it will permeate from a mixture at a rate proportional to its concentration in the mixture, and
- If the chemical does not permeate in pure form, it will not permeate from a mixture.

Additional permeation tests with selected chemical mixtures should be conducted to further test this proposed rule.

SECTION 6

COMPUTERIZED DATABASE AND MODEL FOR PERMEATION PREDICTION

6.1 DESCRIPTION

A computerized version of the permeation database and empirical prediction model was developed for Macintosh computers using SuperCard 1.5 (Silicon Beach Software). The computer system was developed for use by Coast Guard personnel with some basic training in chemistry. In addition to storing the existing Challenge material permeation test results, the computer system allows users to generate predictions using the empirical model described in Section 4.

The system was developed to run on Macintosh Plus and all later versions of Macintosh computers with at least 1 megabyte of RAM. The screen display area has been sized for the Macintosh Plus/SE monitor. The only software requirement is System 6.0.4 or later (available from any Apple dealer). SuperCard is not needed to run the database. The system is divided into two parts: a control program and a data file. The control program is provided in two formats: the master version which allows modification of the data, and the field version which allows "browsing" only. The data file is designed to work with both versions of the control program with no modifications.

6.1.1 Database Structure and Card Format

Each entry in the database is stored on a "card." Thus, for every chemical in the database, there is one card that stores information on the chemical identity, permeation data if available, and permeation model prediction if generated. The card format, illustrated in Figure 10, is segmented into three parts. The first part provides chemical identity information. The second segment provides a permeation data summary using a standard, tabular format. The third segment reports the permeation model prediction, if generated and stored, also using a standard format. Data for all replicates and other temperatures are entered on the Expanded Data segment of the card shown in Figure 11. The Expanded Data segment of the card is accessed from the permeation data summary segment of the card.

Information available for each chemical stored in the database will vary. For example, some chemicals have permeation data for both Challenge 5100 and Challenge 5200 and at several temperatures, while others may have data for only one material at one temperature. Also, some chemicals will have both permeation data and a model prediction, others may have only model predictions. All available information has been included (i.e., no data were excluded as apparent outliers or because of conflicting results) and reported using the standard card format.

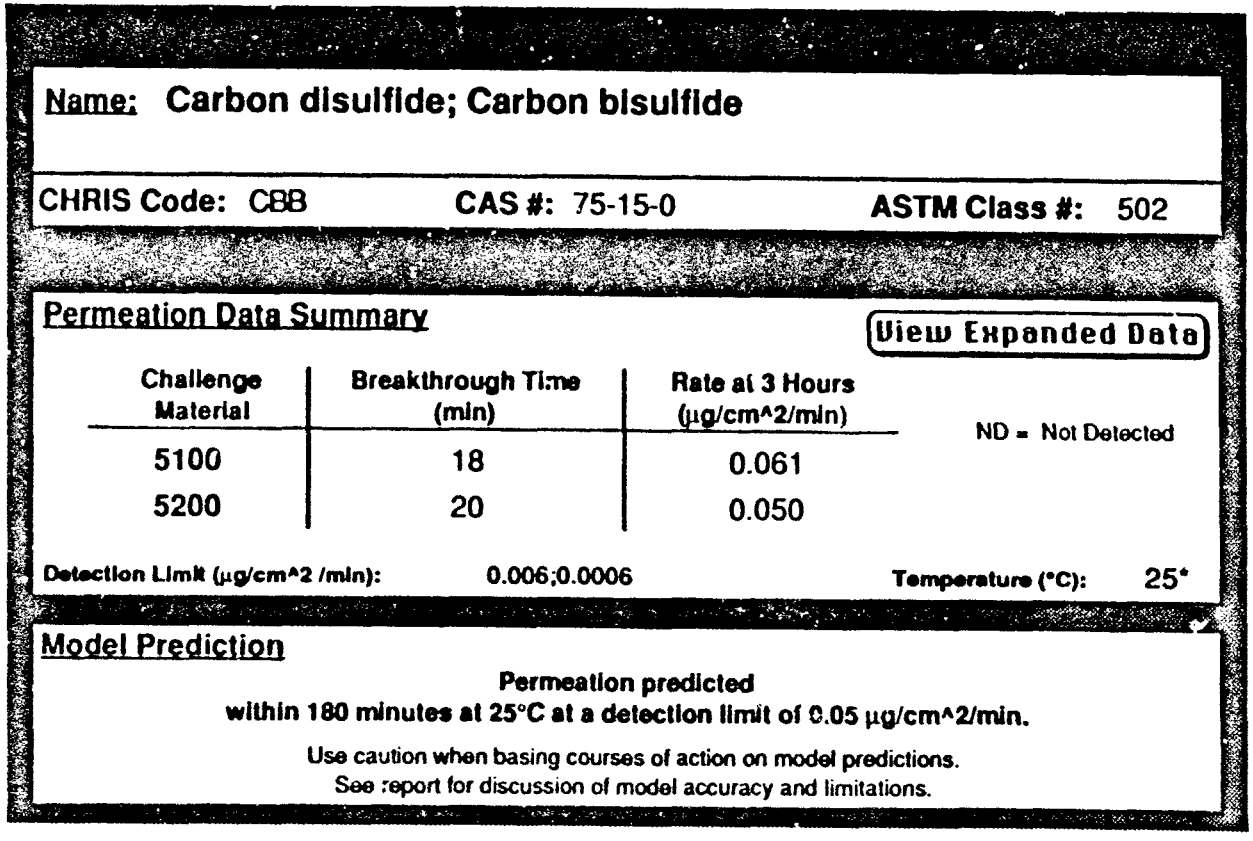
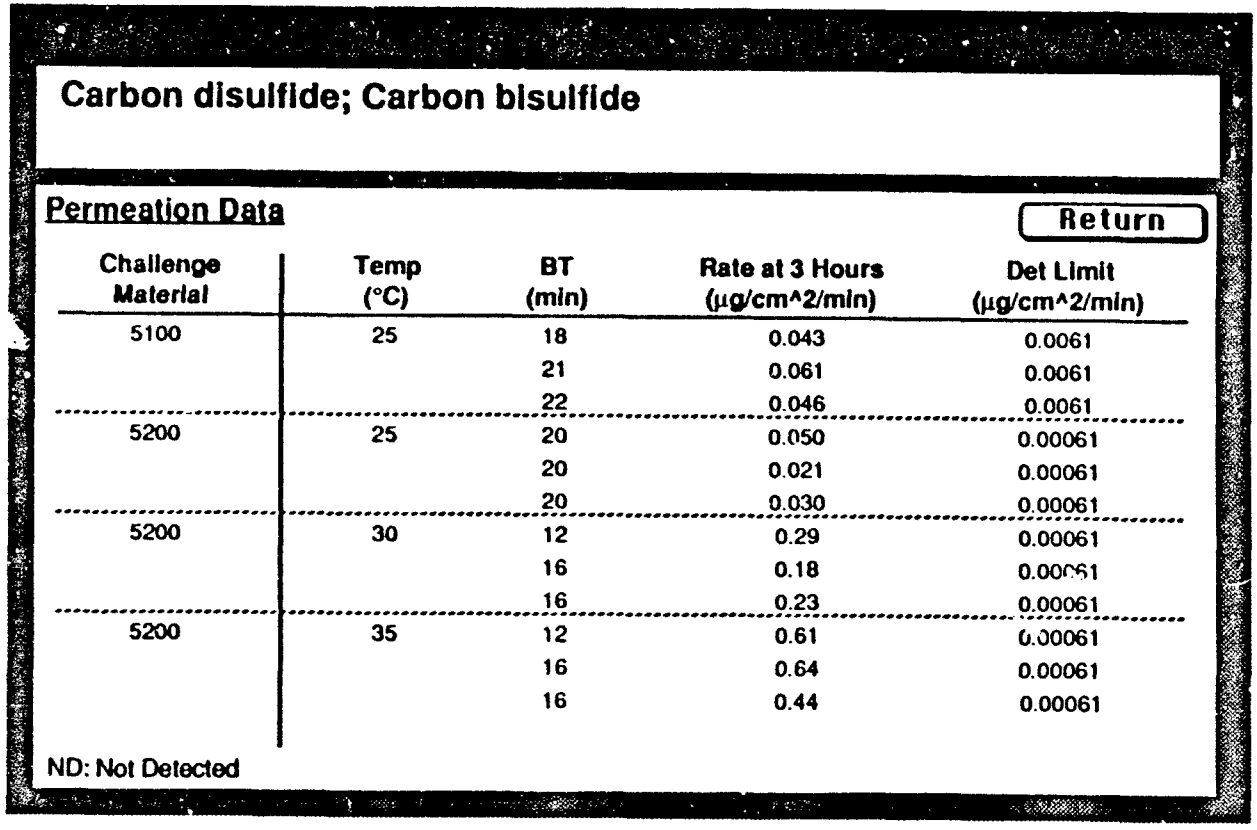


Figure 10. Example of permeation model and database card format.



Carbon disulfide; Carbon bisulfide

Permeation Data

Return

Challenge Material	Temp (°C)	BT (min)	Rate at 3 Hours (µg/cm^2/min)	Det Limit (µg/cm^2/min)
5100	25	18	0.043	0.0061
		21	0.061	0.0061
		22	0.046	0.0061
5200	25	20	0.050	0.00061
		20	0.021	0.00061
		20	0.030	0.00061
5200	30	12	0.29	0.00061
		16	0.18	0.00061
		16	0.23	0.00061
5200	35	12	0.61	0.00061
		16	0.64	0.00061
		16	0.44	0.00061

ND: Not Detected

Figure 11. Example of expanded data card format.

6.1.2 System Operation

System features include capabilities to search the database, run the permeation prediction model, enter data or model predictions into the database (access to this feature is restricted), and print entries from the database. Standard Macintosh procedures are followed to select options from the menu list provided across the top of the screen display area. The menu options include:

- FILE – to print a single entry, to print the all database entries, and to quit from the system
- EDIT – to create/edit a new entry and to delete an existing entry (access to this option is limited)
- SEARCH – to search the database by chemical name or partial name, by CHRIS code, or by CAS number
- MODEL – to run permeation prediction model
- HELP – to access help information on operation of the data base system

6.1.3 Information Required to Run the Model

The computerized model was developed to be easy to use but does require basic chemistry training for proper use. As described in Section 4, the empirical model involves a set of rules or questions regarding the structure and size of the chemical. Therefore, before running the model, the structure of the chemical must be known so that the functional groups present and the number of atoms in the structure can be identified.

The computer system asks a series of questions regarding the chemical structure which the user answers by selecting from the options provided on screen. Most questions involve a Yes or No answer. As each question is answered, the computer selects the next question to ask based on the previous answer. The permeation prediction model ultimately leads to one of two predictions. If permeation is predicted to occur, the following message will be displayed:

Permeation predicted
within 180 minutes at 25°C at a detection limit of 0.05 $\mu g/cm^2$-min.

If no permeation is predicted to occur, the message below will be displayed:

No permeation predicted
within 180 minutes at 25°C at a detection limit of 0.05 $\mu g/cm^2$-min.

The master version of the computer system then provides the option to save the model prediction. Access to this capability is prevented in the field version.

6.2 APPLICABILITY AND LIMITATIONS

It is important to recognize that the permeation model predictions are intended only as guidance. As described throughout this report, the model was developed using the available data set and should be refined as new permeation data become available. Caution should be used when relying solely on permeation model predictions. If there are concerns regarding potential exposures to a specific chemical, permeation testing should be performed.

SECTION 7

CONCLUSIONS AND RECOMMENDATIONS

The permeation resistance of Challenge 5100 and Challenge 5200 has been widely tested and the results indicate that these materials are effective barriers to a broad range of chemicals and chemical mixtures. The materials appear to provide comparable barriers although the Challenge 5100 material may be a slightly better barrier. When permeation was observed, it was shown to follow a simple Fickian diffusion mechanism with a constant diffusion coefficient. However, no quantitative predictive model based on the Fick's law approach was developed however. Also, no definitive conclusions could be reached regarding the effect of temperature on the permeation resistance of the Challenge materials based on the limited data set available.

An empirical model or rule system was developed that enables predictions as to whether permeation will be detected within three hours at 25°C based on the structure and size of the chemical of interest. Based on a smaller set of data, the permeation of mixtures or the components thereof was found to behave similarly to the results for the chemicals tested individually. If a chemical permeates the Challenge material as a pure chemical then it will permeate from a mixture. Conversely, if a chemical does not permeate in pure form then it will not permeate from a mixture.

A computerized version of the permeation data base and prediction model was developed for use by personnel with minimal permeation or chemistry training. The computer system should facilitate thorough and efficient reviews of existing data and assessments of probable permeation behavior by field (or other) users who must make clothing selection decisions. Although use of the model was targeted as an aid for making clothing selection decisions, it is also useful to focus decisions regarding priority chemicals and mixtures for future testing.

Further research should be undertaken to address some of the uncertainties in the data set, the predictive model described herein, and other approaches being evaluated to predict the permeation behavior. Specific recommendations include:

- A trial implementation of the computerized permeation database and predictive model should be undertaken in the field to evaluate the product's usefulness and identify ways to optimize the product to better meet Coast Guard's needs.

- Future permeation tests, if performed, should be conducted so that chemical breakthrough is determined at a single, normalized permeation detection rate, if feasible, as is now being proposed as a revision to ASTM Method F739. Use of a standard permeation detection rate would eliminate some of the difficulties in comparing the present data set.

- Permeation tests with additional chemical mixtures should be undertaken to further validate the mixture permeation rule. Validation of this rule is important because it would eliminate the need to test infinite numbers of chemical mixtures if the behavior can be predicted using only the pure chemical results.

- Selected permeation tests at elevated temperatures should be repeated to confirm the results reported to date and to better understand the effect of temperature on the permeation resistance of the Challenge materials.

- The computerized permeation database should be updated as more data are generated and the predictive model should be continually tested as new data become available to expand and improve the prediction accuracy. Also, further development of a Fick's law based model should be pursued if a quantitative model to predict permeation as a function of time is desired.

- In the long term, similar computer databases and predictive models could be developed to address other important components of the Coast Guard CRS (e.g., glove materials, faceshield material) or alternative materials for the encapsulating suit fabric that may adopted at a later date. Development of such databases and models provide a better understanding of the barrier properties of critical materials and help to focus priorities for testing.

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APPENDIX A

CHALLENGE 5100 AND CHALLENGE 5200 PERMEATION TEST RESULTS AT 25°C

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Acetaldehyde	ND	ND	> 180							
Acetic Acid	35.460	1.7178	> 240							
Acetic Anhydride	0.570	0.0396	> 180							
Acetone	1.160	0.0469	> 210							
Acetone (27C) +	0.001	0.00004	71	1.630 (3hr)	44	1.3000	104	1.2000	64	2.4000
Acetone Cyanohydrin	2.740	0.1881	> 192							
Acetonitrile	ND	ND	> 270							
Acetonitrile +	1.000	0.0331	> 180							
Acetophenone (USCG R&DC)	ND	ND	> 5520							
Acetyl Bromide	0.200	0.0198	> 282							
Acetyl Chloride	35.460	2.2455	> 186							
Acrolein	0.120	0.0054	41	0.033 (ss)	44	0.0395	38	0.0268		
Acrylic Acid	0.860	0.0500	> 180							
Acrylonitrile	0.460	0.0049	65	0.014 (ss)	54		76	0.0143		
Adiponitrile	0.300	0.0261	> 186							
Allyl Alcohol	1.130	0.0529	> 840							
Allyl Amine	0.800	0.0368	> 210							
Allyl Bromide	0.010	0.0010	> 240							
Allyl Chloride	0.160	0.0025	134	0.011 (ss)	102	0.0107	166	0.0103		
Allyl Chloride	0.060	0.0037	143	0.013 (6hr)	136	0.0098	116	0.0210	176	0.0068
Allyl Cyanide	0.400	0.0216	> 240							
Allyl Isothiocyanate	1.000	0.0800	> 258							
Allyl Mercaptan	0.020	0.0012	> 600							
Ammonia (Gas) +	0.040	0.0005	> 180							
Ammonium Hydroxide +	2.000	0.0565	?	(3hr)	30	26.6667	> 180		> 180	
Ammonium Hydroxide +	7.200	0.2033	> 180							
Aniline	0.460	0.0346	> 198							
Benzene	0.050	0.0032	> 192							
Benzoyl Chloride	0.020	0.0023	> 960							

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

Chemical+	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Benzyl Chloride	0.110	0.0112	> 192							
Bromine (Gas)	0.530	0.0683	> 198							
Butanol	0.320	0.0191	> 936							
2-Butanol	0.240	0.0144	> 300							
t-Butanol	0.200	0.0120	> 180							
2-Butoxyethanol	0.040	0.0038	> 258							
Butyl Acetate	0.250	0.0234	> 180							
Butyl Acrylate	0.220	0.0227	> 180							
Butylamine	0.320	0.0189	> 180							
Butyraldehyde	0.290	0.0169	> 450							
Carbon Disulfide	0.100	0.0061	20	0.050 (ss)	22	0.0460	21	0.0608	18	0.0432
Carbon Tetrachloride	0.290	0.0360	> 180							
Chlordane, 25%	0.260	0.0860	> 204							
Chlorobenzene	0.200	0.0182	> 180							
Chloroform	0.190	0.0183	> 216							
Chloropicrin (Trichloronitromethane)	1.800	0.2387	> 186							
Chloroprene (2-Chloro-1,3-Butadiene)	0.030	0.0021	179	0.005 (ss)	192	0.0025	184	0.0032	160	0.0087
Chlorosulfonic Acid	0.500	0.0470	> 180							
Creosote	0.320	*	> 1086							
m-Cresol	0.030	0.0026	> 240							
Crotonaldehyde	0.620	0.0351	> 186							
Cumene Hydroperoxide	1.200	0.1471	> 210							
Cyclohexane	0.250	0.0170	> 204							
Cyclohexanol	0.040	0.0032	> 240							
Cyclohexanone	0.020	0.0016	> 210							
Cyclohexylamine	0.020	0.0016	> 240							
1,2-Dibromoethane	0.100	0.0152	> 204							
Dibromomethane +	0.050	0.0070	> 180							
Dibutyl Phthalate	0.020	0.0045	> 288							

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
o-Dichlorobenzene	0.010	0.0012	> 870							
p-Dichlorobenzene	0.020	0.0024	> 240							
1,2-Dichloroethane	0.090	0.0072	> 342							
1,2-Dichloroethylene	0.010	0.0008	15	1.079 (ss)	20	0.1933	4	2.9333	20	0.1115
1,2-Dichloroethylene	0.010	0.0008	23	0.130 (ss)	21	0.1417	24	0.1177		
1,2-Dichloroethyl Ether	ND	ND	> 180							
Dichloromethane	0.270	0.0042	51	0.020 (ss)	47	0.0228	50	0.0161	55	0.0212
Dichloromethane (USCG R&DC)	0.030	*	61		54		65		63	
1,2-Dichloropropane	0.310	0.0283	> 186							
1,3-Dichloropropene	0.170	0.0152	> 180							
Diethanolamine	ND	ND	> 180							
Diethylamine (USCG R&DC)	ND	ND	> 270							
Diethylenetriamine	0.900	0.0749	> 1200							
Diisopropylamine	0.390	0.0318	> 672							
2,3-Dimethyl-2-Butene	0.020	0.0014	> 300							
Dimethylformamide (USCG R&DC)	ND	ND	> 192							
Dimethyl Sulfate	1.520	0.1547	> 180							
1,4-Dioxane	0.380	0.0270	> 180							
Di-n-Propylamine	0.220	0.0180	> 204							
Epichlorohydrin	0.750	0.0560	> 180							
1,2-Epoxy Butane	0.070	0.0041	> 180							
Ethanol	2.860	0.1063	> 180							
Ethion 4	0.030	0.0093	> 288							
2-Ethoxy Ethanol	0.050	0.0036	> 300							
Ethyl Acetate	0.490	0.0348	> 258							
Ethyl Acrylate	1.720	0.1369	> 1020							
Ethylamine (70%)	0.740	0.0269	> 180							
Ethyl Benzene	0.140	0.0120	> 180							
Ethylene +	0.090	0.0020	> 180							

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Ethylene Cyanohydrin	0.400	0.0229	> 228							
Ethylenediamine	2.780	0.1348	> 192							
Ethylene Glycol	2.630	0.1317	> 1008							
Ethylene Sulfide	0.300	0.0145	> 180							
Ethyl Ether	0.130	0.0078	> 180							
Ethyl Ether +	0.010	0.0006	92	0.005 (3hr)	88	0.0060	84	0.0078	104	0.0012
Ethyl Ether (27C) +	0.006	0.0004	117	1.070 (3hr)	124	1.4000	112	0.9000	116	0.9000
Ethyl Vinyl Ether	0.030	0.0017	113	0.008 (3hr)	148	0.0040	92	0.0117	100	0.0075
Formaldehyde, 37%	ND	ND	> 180							
Formic Acid	1.000	0.0371	> 1200							
Freon 12 (Gas) +	3.500	0.3414 ul	?	(3hr)	160	0.0001	> 180		> 180	
Furfural	0.080	0.0062	> 186							
Gasoline	1.650	*	> 894							
Glutaraldehyde (sol'n)	0.430	0.0347	> 216							
Heptane	0.040	0.0032	> 240							
Hexane	0.250	0.0174	> 300							
Hexylene Glycol	0.080	0.0076	> 198							
Hydrazine Hydrate [10217-52-4]	0.900	0.0233	> 192							
Hydrochloric Acid	2.000	0.0588	> 180							
Hydrogen Peroxide, 30%	0.600	0.0165	> 180							
Isobutyl Acetate	0.030	0.0028	> 180							
Isobutanol +	0.040	0.0024	> 180							
Isophorone	0.030	0.0033	> 300							
Isopropanol	1.160	0.0562	> 180							
Isopropyl Acetate	0.100	0.0082	> 240							
Isopropylamine	1.570	0.0749	> 180							
Isopropyl Ether	0.010	0.0008	> 180							
Malathion, 50%	1.030	0.2745	> 186							
Mesityl Oxide	0.300	0.0238	> 240							

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2-min)		Average BT (min)	Average Reported rate** (ug/cm^2-min)		Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Methacrylonitrile	0.290	0.0157	>	180								
Methanol	4.070	0.1052	>	852								
Methyl Acrylate	0.120	0.0083	>	180								
Methyl Bromide (Gas) +	0.010	0.0008	ul	27	0.0004	(as)	28	0.0002	28	0.0005	24	0.0005
2-Methyl-2-Butene	0.110	0.0062	>	180								
Methyl Ethyl Ketone	0.650	0.0378	>	180								
Methyl Isobutyl Ketone	3.900	0.3151	>	180								
Methyl Isocyanate (NIOSH)	0.260	*		28		(ac)	28					
Methyl Methacrylate	0.190	0.0132	>	186								
Methyl Parathion	0.150	0.0319	>	186								
Methyl Vinyl Ketone	0.050	0.0028	>	180								
Morpholine	0.020	0.0014	>	960								
Naled	ND	ND	>	204								
Naphthalene	ND	ND	>	792								
Naphtha, Stoddard Solvent	0.040	*	>	480								
Nitric Acid	0.200	0.0102	>	180								
Nitrobenzene	0.080	0.0079	>	180								
Nitromethane +	0.260	0.0128	>	180								
2-Nitropropane	0.590	0.0424	>	180								
Oleum (Sulfuric Acid, Fuming)	0.200	0.0158	>	180								
Parathion	0.090	0.0211	>	180								
Petroleum Ether	4.550	*	>	204								
Phenol	0.030	0.0023	>	180								
Phosphoric Acid	0.500	0.0395	>	180								
Phosphorus Oxychloride	0.500	0.0619	>	180								
Phosphorus Trichloride	0.500	0.0554	>	180								
Polychlorinated Biphenyls	0.020	*	>	180								
Potassium Hydroxide	1.000	0.0453	>	180								
Propanol	0.760	0.0368	>	180								

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2 min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Propionic Acid	0.310	0.0185	> 180							
Propyl Acetate	0.200	0.0165	> 240							
Propylamine	0.740	0.0353	> 612							
Propylene (Gas) +	0.010	0.0003	61	0.0003 (ss)	60	0.0002	48	0.0005	76	0.0002
Propylene Oxide	0.680	0.0080	154	0.021 (ss)	137	0.0238	170	0.0182		
Pyridine	0.020	0.0013	> 240							
Silicon Tetrachloride	0.500	0.0685	> 180							
Sodium Hydrosulfide	0.500	0.0226	> 180							
Sodium Hydroxide, 50% (USCG)	ND	ND	> 4260							
Sodium Hydroxide, 50%	0.500	0.0161	> 180							
Styrene	0.050	0.0042	> 240							
Sulfuric Acid, 95%	0.200	0.0158	> 180							
Sulfur Monochloride	0.500	0.0545	> 180							
1,1,2,2-Tetrachloroethane	0.230	0.0311	> 912							
Tetrachloroethylene	0.110	0.0147	> 624							
Tetrachloroethylene (USCG R&DC)	ND	ND	108	(nc)	108					
Tetrachloroethylene (27C) +	0.001	0.0001	7	(3hr)	180		8	33.0000	44	3.0000
Tetrahydrofuran (USCG R&DC)	ND	ND	> 330							
1,1,1-Trichloroethane	0.600	0.0646	> 180							
Trichloroethylene	0.070	0.0017	148	0.031 (ss)	143	0.0340	156	0.0272	146	0.0318
Trichloroethylene	0.010	0.0011	138	0.031 (6hr)	155	0.0148	140	0.0233	120	0.0540
Toluene	0.060	0.0045	> 180							
Toluene-2,4-Diisocyanate	0.690	0.0969	> 198							
o-Toluidine	0.430	0.0372	> 198							
Turpentine	0.030	*	> 216							
Vinyl Acetate	0.210	0.0036	106	0.059 (ss)	74	0.0550	137	0.0622		
Vinyl Methyl Ether +	0.540	0.0253	60	2.242 (3hr)	60	3.5833	60	2.3667	60	0.7750
Vinylidene Chloride	0.490	0.0383	> 180							
Vinylidene Chloride +	0.010	0.0008	51	0.022 (3hr)	52	0.0117	52	0.0110	48	0.0433

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

Chemical+	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Vinylidene Fluoride +	0.700	0.0361	> 180							
Xylenes	0.130	0.0111	> 180							
Xylenol (Dimethylphenol)	ND	ND	> 198							

\+ Received after initial model development effort.

* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (*) could not be converted. ND indicates not determined.
Note: ul indicates that the MDR and the reported rate are reported in units of ul/cm^2-min.

** Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parenthesis when known. (ss) indicates a steady-state permeation rate value. (nc) indicates that no permeation time curve was available.

Source: U.S. Coast Guard Research and Development Center
Testing Laboratory: Texas Research International (unless otherwise noted)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

Chemical+	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Acetone	1.000	0.0404	> 180							
Acetone (27C) +	0.010	0.0004	116	0.0004 (3hr)	116	0.0002	116	0.0005	116	0.0005
Acetone (27C) +	0.001	0.00004	> 180							
Acetone (ChemFab) +	0.100	*	> 300							
Acetonitrile	2.000	0.0662	> 180							
Acetonitrile (ChemFab) +	2.000	*	> 300							
Acetyl Chloride +	0.020	0.0013	> 180							
Allyl Chloride +	0.030	0.0019	56	0.2833 (3hr)	68	0.2867	64	0.1498	36	0.4133
Ammonia (Gas)	0.300	0.0041	31	0.1144 (ss)	36	0.0783	24	0.1583	32	0.1067
Ammonia (Gas) +	0.070	0.0010 ul	25	0.2378 (3hr)	18	0.2683	23	0.2867	35	0.1583
Ammonia (Gas) (27C) +	0.030	0.0004 ul	32	0.1490 (ss)	32	0.1200	32	0.2183	32	0.1100
Ammonia (Gas) (ChemFab) +	0.100	*	> 300							
Ammonium Hydroxide +	0.250	0.0071	> 180							
Ammonium Hydroxide (27C) +	7.200	0.2033	120	0.3390 (3hr)	120	0.2500	120	0.4500	120	0.3167
Ammonium Sulfide, 20% +	1.000	0.0412	> 180							
Asphalt +	1.000	*	> 180							
Benzaldehyde +	0.010	0.0009	> 180							
Benzonitrile +	0.010	0.0008	> 180							
Benzonitrile +	0.020	0.0017	> 180							
Benzyl Bromide +	0.010	0.0014	> 180							
Benzylamine +	0.010	0.0009	> 180							
Bromoethane	0.010	0.0009	120	0.0281 (3hr)	144	0.0245	84	0.0325	132	0.0272
Bromochloromethane	0.030	0.0031	98	0.0188 (7hr)	93	0.0188	109	0.0147	93	0.0230
1,3-Butadiene (Gas)	0.068	0.0030	5	0.0389 (5hr)	8	0.0240	4	0.0375	4	0.0552
1,3-Butadiene (Gas) +	0.010	0.0004 ul	24	0.0795 (3hr)	24	0.1300	24	0.0700	24	0.0383
Butane (Gas)	0.300	0.0141	> 180							
2-Butene (Gas) (27C) +	0.040	0.0018	55	0.1300 (3hr)	72	0.1000	36	0.2000	56	0.1000
Butyl Chloride	0.070	0.0052	> 180							
Butylamine +	0.010	0.0006	> 180							

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
iso-Butyronitrile +	0.310	0.0173	> 180							
Carbon Disulfide	0.010	0.0006	20	0.0335 (3hr)	20	0.0497	20	0.0208	20	0.0300
Carbon Disulfide (ChemFab) +	0.300	*	143	0.0500 (nc)						
Cetyltrimethylammonium Chloride +	0.100	0.0258	> 180							
Chlorine (Gas) +	1.000	0.0572	70	0.0182 (nc)	90	0.0138	60	0.0267	60	0.0143
Chlorine (Gas) +	38.000	*	60	170.33 (nc)	30	320.00	90	140.00	60	51.0000
Chlorine (Gas) (ChemFab) +	0.300	*	> 300							
Chloroacetone +	0.010	0.0007	> 180							
Chloroacetyl Chloride +	0.020	0.0018	> 180							
4-Chlorobutyronitrile +	0.030	0.0025	> 180							
Chloroethane +	0.070	0.0036	60	0.6330 (nc)	68	0.3667	52	1.2500	60	0.2833
2-Chloroethanol +	0.020	0.0013	> 180							
Chloromethane (ChemFab) +	0.260	*	21	0.7600 (nc)						
Chloromethyl Methyl Ether +	0.010	0.0006	> 180							
1-Chloropropane	2.000	0.1267	260	0.2367 (7hr)	285	0.1433	269	0.2350	225	0.3317
Chromyl Chloride +	0.100	0.0125	> 180							
Cresols +	0.010	0.0009	> 180							
Cumene +	0.010	0.0010	> 180							
Cyanogen (Gas) +	0.500	0.0210	30	0.0600 (nc)						
Cyanogen Bromide (Solid) +	1.000	0.0855	> 180							
Cyanogen Chloride (Gas) +	0.500	0.0248	> 180							
Cyclopropane (Gas) +	0.020	0.0007 ul	92	0.0008 (3hr)	96	0.0003	72	0.0015	108	0.0005
Cyclopropane (Gas) (27C) +	0.002	0.0001	78	0.0008 (3hr)	76	0.0008	80	0.0013	80	0.0002
Decyl Aldehyde +	0.010	0.0013	> 180							
Dibromomethane	0.030	0.0042	> 180							
1,3-Dichloro-2-Butene +	0.010	0.0010	> 180							
1,2-Dichloroethylene +	0.010	0.0008	24	0.3578 (nc)	28	0.2850	28	0.4050	16	0.3833
cis-1,2-Dichloroethylene	0.010	0.0008	69	0.1550 (3hr)	56	0.2200	80	0.0967	72	0.1483
trans-1,2-Dichloroethylene +	0.010	0.0008	19	1.3967 (ss)	19	1.4317	19	1.4700	19	1.2883

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Dichloromethane (27C) +	0.007	0.0005	83	3.6700 (3hr)	84	4.0000	88	3.0000	76	4.0000
Dichloromethane +	0.005	0.0003	64	0.2630 (3hr)	68	0.2300	52	0.3700	72	0.1900
Dichloromethane (ChemFab) +	0.100	*	64	0.1200 (nc)						
Diethylamine (ChemFab) +	0.400	*	> 300							
Dimethyl Acetamide*	0.010	0.0007	> 180							
Dimethylformamide (ChemFab) +	0.700	*	> 300							
Dimethylhydrazine +	0.090	0.0044	> 180							
Dimethyl Sulfide (Methyl Sulfone) +	0.010	0.0008	95	0.0005 (3hr)	116	0.0005	76	0.0005	92	0.0005
Dimethyl Sulfide (Methyl Sulfone) +	0.010	0.0008	48	0.0002 (3hr)	60	0.0002	40	0.0002	44	0.0003
Dimethyl Sulfoxide	0.010	0.0006	> 180							
Diphenyldichlorosilane +	3.000	0.6123	> 180							
1-Dodecanethiol +	1.000	0.1630	> 180							
Ethane +	1.000	0.0243	> 180							
Ethanethiol +	0.020	0.0010	65	0.0028 (3hr)	60	0.0030	76	0.0025	60	0.0030
Ethanethiol (27C) +	0.003	0.0002	83	15.3300 (3hr)	88	4.0000	88	16.0000	72	26.0000
Ethyl Acetate	0.010	0.0007	> 180							
Ethyl Acetate (ChemFab) +	0.100	*	> 300							
Ethyl Acrylate	0.050	0.0040	> 180							
Ethyl Chloroformate +	0.200	0.0175	> 180							
Ethyl Ether (27C)	0.010	0.0006	127	0.3761 (20hr)	104	0.4050	136	0.3033	140	0.4200
Ethyl Ether (27C) +	0.010	0.0006	92	0.0080 (3hr)	92	0.0143	96	0.0035	88	0.0072
Ethyl Ether (27C) +	0.003	0.0002	149	2.1000 (3hr)	144	4.9000	156	0.9000	148	0.5000
Ethyl Ether (27C) +	0.010	0.0006	40	173.33 (3hr)	44	130.00	36	220.00	40	170.00
2-Ethylhexanal +	0.010	0.0010	> 180							
2-Ethylhexylacrylate +	0.010	0.0015	> 180							
Ethyl Methacrylate +	0.010	0.0009	> 180							
Ethyl Vinyl Ether	0.020	0.0012	23	0.6694 (3hr)	40	0.3933	8	0.5517	20	1.0633
Ethyl Vinyl Ketone +	0.060	0.0041	> 180							
Ethyleneimine +	0.020	0.0007	> 180							

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

Chemical+	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Ethylene Oxide (Gas) +	3.000	0.1066	57	0.7250 (3hr)	68	0.8250	60	0.8483	44	0.5017
Ethylene Oxide (Gas) +	0.650	0.0231	25	0.1420 (3hr)	20	0.1418	24	0.1683	32	0.1160
Ethylene Oxide (Gas) (ChemFab) +	0.340	*	64	0.7600 (ac)						
Freon 11 (Trichlorofluoromethane) +	0.500	0.0554	> 180							
Freon 12 (Dichlorodifluoromethane)	0.100	0.0098	> 180							
Freon 21 (Dichlorofluoromethane) +	3.000	0.2491	> 180							
Freon 22 (Chlorodifluoromethane) +	3.000	0.2093	> 180							
Gasoline JP-4 +	0.100	*	> 180							
Hexanal +	0.020	0.0016	> 180							
Hexane +	0.100	0.0070	> 300							
Hexene +	0.010	0.0007	> 180							
Hydrazine (ChemFab) +	0.760	*	> 480							
Hydrobromic Acid (Gas) +	10.000	0.6527	> 180							
Hydrogen Chloride (Gas) (ChemFab)	0.040	*	> 480							
Hydrogen Cyanide (Gas) (ChemFab)	0.050	*	> 480							
Hydrogen Sulfide (Gas) +	0.030	0.0008 ul	4	0.0028 (3hr)	4	0.0017	4	0.0005	4	0.0017
Hydrogen Sulfide (27C) (Gas) +	0.010	0.0003 ul	8	0.0070 (3hr)	8	0.0055	8	0.0077	8	0.0068
Hydrogen Sulfide (Gas) +	0.030	0.0008 ul	15	0.0078 (ac)	20	0.0017	12	0.0133	12	0.0083
2-Hydroxyethyl Acrylate +	0.120	0.0112	> 180							
Isobutylamine +	0.030	0.0018	> 180							
Isobutyraldehyde +	0.010	0.0006	> 180							
Isoprene	0.010	0.0005	9	0.1820 (3hr)	8	0.0615	8	0.1295	12	0.3550
Isovaleraldehyde +	0.010	0.0007	> 180							
Methane +	1.000	0.0129	7	18.0000 (ac)	7	16.0000	6	27.0000	8	11.0000
Methanol (ChemFab) +	0.400	*	> 300							
Methyl Acetate +	0.020	0.0012	112	0.0053 (3hr)	84	0.0072	144	0.0042	108	0.0048
Methyl Acrylate +	7.000	0.4861	7	(3hr)	116	0.7683	112	0.7700	> 180	
Methyl Bromide (Gas) +	0.400	0.0306	21	0.0347 (3hr)	20	0.0367	20	0.0367	24	0.0308
Methyl Bromide (Gas) +	0.020	0.0015 ul	20	0.0065 (3hr)	20	0.0053	20	0.0073	20	0.0067

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

Chemical+	MDL* (ppm)	MDR* (ug/cm^2-min)		Average BT (min)	Average Reported rate** (ug/cm^2-min)		Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Methyl Chloride (Gas) (27C) +	0.060	0.0024	ul	16	0.0020	(ss)	16	0.0020	16	0.0020	16	0.0020
Methyl Chloroformate +	0.050	0.0038		81	0.0120	(3hr)	76	0.0092	76	0.0198	92	0.0068
Methyl Chloroformate (27C) +	0.100	0.0076		95	0.9500	(3hr)	116	0.7500	72	1.2000	96	0.8900
Methyl Ethyl Ketone (ChemFab) +	1.000	*	>	120								
Methyl Iodide+	0.370	0.0424		32	17.2333	(3hr)	32	27.0000	32	10.8000	32	13.9000
Methyl Isocyanate +	0.010	0.0005		92	0.0202	(3hr)	96	0.0207	72	0.0188	108	0.0212
Methyl Vinyl Ketone	0.010	0.0006	>	180								
Methylamine (Gas)	0.200	0.0050	>	180								
Monoethanolamine +	0.010	0.0005	>	180								
Nicotine +	1.000	0.1309	>	180								
Nitric Acid, Red Fuming (ChemFab)	0.100	*	>	480								
Nitric Oxide (Gas) +	1.000	0.0508	ul	30	2.0000							
2-Nitroaniline +	0.100	0.0111	>	180								
4-Nitroaniline +	0.010	0.0011	>	180								
Nitrobenzene (ChemFab) +	1.000	*	>	300								
Nitroethane +	0.010	0.0006	>	180								
Nitrogen Dioxide (Gas) +	0.500	0.0186	ul	4	4.9900	(ss)	4	5.3333	4	6.3500	4	3.2833
Nitrogen Tetroxide (Gas) +	0.080	0.0059	ul	15	13.7600	(ss)	24	16.2000	4	18.7000	16	6.4000
Nitromethane	0.730	0.0359		168	0.0538	(ss)	168	0.0447	168	0.0630	168	0.0537
Nitropropane +	0.700	0.0345	>	180								
o-Nitrotoluene +	0.010	0.0011	>	180								
Nonyl Phenol +	0.100	0.0177	>	180								
Pentachlorophenol +	1.000	0.2149	>	180								
Pentanedione +	0.100	0.0081	>	180								
2,4-Pentanedione +	0.070	0.0057	>	180								
Pentene +	0.010	0.0006		81	0.0440	(ss)	88	0.0500	64	0.0500	92	0.0333
Pentyltrichlorosilane +	0.010	*	>	180								
Perchloric Acid +	0.350	0.0284	>	180								
Phenyldodecane +	1.000	0.1984	>	180								

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL* (ppm)	MDR* (ug/cm^2-min)	Average BT (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Phosgene (Gas) (27C) +	0.500	*	60	0.2000 (nc)	60	0.2000	60	0.2000	60	0.2000
Phosgene (Gas) (ChemFab) +	1.000	*	> 480							
Potassium Hydroxide +	0.500	0.0226	> 180							
Propane +	0.010	0.0004	> 180							
1-Propanethiol +	0.050	0.0031	> 180							
2-Propanethiol +	0.010	0.0006	> 180							
Propiolactone +	0.020	0.0012	> 180							
Propylene Oxide (27C) +	0.010	0.0005	89	0.0001 (3hr)	96	0.0001	96	0.0001	76	0.0002
Sodium Hydroxide +	0.500	0.0161	> 180							
Sodium Hydroxide, 50% (ChemFab)	0.200	*	> 300							
Sulfur Dioxide (Gas) +	47.000	2.4292 ml	60	0.0895 (3hr)	60	0.0717	60	0.1250	60	0.0717
Sulfur Dioxide (Gas) +	1.000	0.0517 ml	40	2.3000 (nc)	30	2.3000	60	2.3000	30	2.3000
Sulfuryl Chloride +	0.010	0.0011	> 180							
Tetrachloroethylene (ChemFab) +	0.200	*	> 300							
Tetraethylenepentamine +	1.000	0.1525	> 180							
Tetrahydrofuran (ChemFab) +	0.100	*	> 300							
Toluene (ChemFab) +	0.100	*	> 300							
1,1,2-Trichloroethane +	0.690	0.0743	> 180							
Trichloroethylene +	0.016	0.0011	49	0.1949 (3hr)	52	0.2017	56	0.1630	40	0.2200
Trichloroethylene (27C) +	0.010	0.0011	72	0.0028 (3hr)	80	0.0022	76	0.0042	60	0.0022
Triethylbenzene +	0.010	0.0013	> 180							
Triethylenetetramine +	0.010	0.0012	> 180							
Trimethylamine +	0.150	0.0072	20		20					
Trimethylamine +	0.014	0.0007	> 180							
Trimethylamine +	0.150	0.0072	25		20		24		32	
Vinyl Acetate	0.020	0.0014	69	0.2522 (nc)	68	0.2433	64	0.3350	76	0.1783
Vinyl Acetate +	0.004	0.0003	73	38.0000 (3hr)	65	50.0000	85	35.0000	69	29.0000
Vinyl Acetate +	0.004	0.0003	109	11.2800 (3hr)	79	25.2000	132	2.1900	124	6.4400
Vinyl Chloride (Gas) +	0.010	0.0005 ml	12	0.0840 (3hr)	12	0.0860	12	0.0952	12	0.0715

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

Chemical +	MDL• (ppm)	MDR• (ug/cm^2-min)	Average BT (min)	Average Reported rate•• (ug/cm^2-min)	Replicate #1 BT (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 BT (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 BT (min)	Replicate #3 Reported rate (ug/cm^2-min)
Vinyl Chloride (Gas) +	0.020	0.0010 ul	7	0.0600 (3hr)	4	0.0800	8	0.0400	8	0.0400
Vinyl Methyl Ether +	33.000	1.5448	28	19.1000 (3hr)	36	7.6500	24	35.0500	24	14.6000
Vinyl Sulfone +	0.010	0.0010	> 180							
Vinylidene Chloride	0.490	0.0383	124	1.0828 (3hr)	120	1.4800	120	0.8800	132	0.8883
Vinylidene Chloride (27C) +	0.010	0.0008	40	0.0860 (3hr)	32	0.1570	40	0.0655	48	0.0352
Vinylidene Chloride +	0.030	0.0023	61	0.0822 (3hr)	64	0.0567	60	0.0900	60	0.1000
Vinylidene Fluoride +	0.040	0.0021	32	0.0760 (3hr)	32	0.0700	32	0.0900	32	0.0700

+ Received after initial model development effort.

• MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (*) could not be converted. ND indicates not determined.
Note: ul indicates MDR and reported rate are in units of ul/cm^2-min, ml indicates MDR and reported rate are in units of ml/cm^2-min.

•• Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parenthesis when known. (ss) indicate a steady-state permeation rate value. (nc) indicates that no permeation time curve was available.

Source: U.S. Coast Guard Research and Development Center
Testing Laboratory: Texas Research International (unless otherwise noted)
(USCG R&DC=U.S. Coast Guard Research and Development Center, ChemFab=Chemical Fabrics Corporation)

APPENDIX B

CHALLENGE 5200 PERMEATION TEST RESULTS AT ELEVATED TEMPERATURES

TABLE B-1. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 30C

Chemical	MDL* (ppm)	MDR* (ug/cm^2-min)	Average Break. time (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 Break. time (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 Break. time (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 Break. time (min)	Replicate #3 Reported rate (ug/cm^2-min)
Acetone	0.01	0.0004	> 210							
Acrolein	0.17	0.0077	56	0.095 (nc)	48	0.102	60	0.071	60	0.112
Acrylonitrile	0.04	0.0017	76	0.028 (nc)	84	0.024	68	0.032	76	0.028
Allyl Chloride	0.05	0.0031	56	0.035 (nc)	52	0.030	56	0.051	60	0.024
Carbon Disulfide	0.01	0.0006	15	0.234 (nc)	16	0.178	16	0.230	12	0.293
Dichloromethane	0.01	0.0007	43	0.037 (nc)	48	0.028	36	0.040	44	0.043
Dichloromethane	0.03	0.0021	52	0.072 (nc)	49	0.091	53	0.062	53	0.063
Diethylamine	0.04	0.0024	> 1182							
Dimethylformamide	0.02	0.0012	> 240							
Ethyl Acetate	0.02	0.0014	> 300							
Hexane	0.10	0.0070	> 300							
Methanol	0.25	0.0065	> 300							
Nitrobenzene	0.10	0.0099	> 180							
Propylene Oxide	0.04	0.0019	108	0.008 (nc)	108	0.009	96	0.013	120	0.003
Propylene Oxide	0.01	0.0005	115	0.003 (3hr)	108	0.004	112	0.004	124	0.002
Tetrachloroethylene	0.01	0.0013	> 240							
Tetrahydrofuran	0.19	0.0111	> 276							
Toluene	0.01	0.0007	> 300							
Trichloroethylene	0.01	0.0011	84	0.139 (nc)	80	0.126	80	0.122	92	0.168
Vinyl Acetate	0.03	0.0021	101	0.089 (nc)	98	0.104	98	0.083	107	0.080

* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area.

** Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (nc) indicates that no permeation-time curve was available.

Source: U.S. Coast Guard Research and Development Center
Testing Laboratory: Texas Research International

TABLE B-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 35C

Chemical	MDL* (ppm)	MDR* (ug/cm^2-min)	Average Break. time (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 Break. time (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 Break. time (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 Break. time (min)	Replicate #3 Reported rate (ug/cm^2-min)
Acetone	0.01	0.0004	67	0.015 (4hr)	32	0.016	80	0.014	88	0.015
Acrolein	0.04	0.0018	23	0.679 (4hr)	20	0.258	22	0.218	27	1.562
Acrylonitrile	0.20	0.0086	110	0.071 (3hr)	93	0.085	117	0.067	121	0.060
Allyl Chloride	0.13	0.0080	236	0.530 (7hr)	229	0.648	237	0.552	241	0.390
Carbon Disulfide	0.01	0.0006	16	0.559 (3hr)	12	0.608	16	0.635	20	0.435
Chloroform	0.02	0.0019	> 240							
Dichloromethane	0.04	0.0027	43	0.188 (3hr)	44	0.220	40	0.175	44	0.170
Diethylamine	0.07	0.0041	> 180							
Dimethylformamide	0.01	0.0006	> 180							
Ethyl Acetate	0.01	0.0007	179	0.003 (6hr)	152	0.004	204	0.003	180	0.004
Hexane	0.02	0.0014	> 180							
Methanol	0.61	0.0158	88	0.063 (nc)	72	0.077	88	0.070	104	0.043
Nitrobenzene	0.07	0.0070	> 180							
n-Propylamine	0.83	0.0396	> 180							
Propylene Oxide	0.06	0.0028	111	0.043 (3hr)	88	0.060	124	0.040	120	0.030
Tetrachloroethylene	0.01	0.0013	236	0.058 (4hr)	236	0.058	236	0.072	236	0.043
Tetrahydrofuran	0.42	0.0244	> 180							
Toluene	0.01	0.0007	> 180							
Trichloroethylene	0.01	0.0011	76	0.337 (3hr)	68	0.325	84	0.338	76	0.348
Vinyl Acetate	0.01	0.0007	60	0.614 (4hr)	52	0.643	52	0.842	76	0.357

* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area.

** Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (nc) indicates that no permeation-time curve was available.

Source: U.S. Coast Guard Research and Development Center
Testing Laboratory: Texas Research International

TABLE B-3. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 40C

Chemical	MDL* (ppm)	MDR* (ug/cm^2-min)	Average Break. time (min)	Average Reported rate** (ug/cm^2-min)	Replicate #1 Break. time (min)	Replicate #1 Reported rate (ug/cm^2-min)	Replicate #2 Break. time (min)	Replicate #2 Reported rate (ug/cm^2-min)	Replicate #3 Break. time (min)	Replicate #3 Reported rate (ug/cm^2-min)
Allyl Chloride	0.07	0.0043	79	0.512 (3hr)	64	0.548	88	0.517	84	0.470
Dichloromethane	0.03	0.0021	29	0.269 (3hr)	28	0.303	32	0.230	28	0.273
Epichlorohydrin	0.18	0.0134	149	0.221 (3hr)	132	0.247	140	0.227	176	0.188
Ethyl Chloroformate	0.01	0.0009	108	0.259 (3hr)	116	0.725	104	0.033	104	0.018
Methacrylonitrile	0.25	0.0135	> 180							
Nitrobenzene	0.02	0.0020	> 180							
Tetrachloroethylene	0.01	0.0013	201	0.097 (3hr)	164	0.113	176	0.125	263	0.052
Trichloroethylene	0.01	0.0011	81	0.477 (ss)	68	0.452	80	0.567	96	0.412
Vinyl Acetate	0.02	0.0014	69	0.252 (8hr)	68	0.243	64	0.335	76	0.178

* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area.

** Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (ss) indicates a steady-state permeation rate.

Source: U.S. Coast Guard Research and Development Center
Testing Laboratory: Texas Research International

APPENDIX C

CHEMICAL MIXTURE PERMEATION TEST RESULTS
(TEXAS RESEARCH INTERNATIONAL)

TABLE C-1. CHEMICAL MIXTURE PERMEATION TEST RESULTS

Mix. #	Mixture Component #1	Mixture Component #2	Mixture Component #3	Material		Component #1 MDL (ppm)	Component #1 BT (min)	Component #2 MDL (ppm)	Component #2 BT (min)	Component #3 MDL (ppm)	Component #3 BT (min)
1	Acetone	Vinyl Acetate	--	5100		0.01	> 180	0.01	120		
2	Acetonitrile	Chlorobenzene	--	5100		0.02	93	0.01	> 180		
3	Acetonitrile	1,2-Dichloroethane	--	5100		0.02	85, > 180	0.01	> 180		
4	Acetonitrile	Nitrobenzene	--	5100		0.02	80	0.01	> 180		
5	Acetonitrile	Chlorobenzene	Nitrobenzene	5100		0.02	80	0.01	> 180	0.01	> 180
6	Acrylonitrile	Trichloroethylene	--	5100		0.01	120-140	0.01	60-80		
7	Carbon Disulfide	Dichloromethane	(75%) --	5100	**	0.02	12	0.02	12		
8	Carbon Disulfide	Dichloromethane	(50%) --	5100	**	0.55	17	0.55	17		
9	Carbon Disulfide	Dichloromethane	(25%) --	5100	**	0.03	16	0.03	16		
10	Carbon Disulfide	Dimethylformamide	--	5100		0.01	12	0.01	> 180		
11	Chlorobenzene	Dichloromethane	--	5100		0.01	> 180	0.02	81		
12	Dichloromethane	Nitrobenzene	--	5100		0.02	56	0.01	> 180		
13	Dichloromethane	Trichloroethylene	(75%) --	5100	**	0.06	47	0.06	47		
14	Dichloromethane	Trichloroethylene	(50%) --	5100	**	0.03	68	0.03	68		
15	Dichloromethane	Trichloroethylene	(25%) --	5100	**	0.05	105	0.05	105		
16	Acetone	Chlorobenzene	--	5200	*	0.10	> 180	0.10	> 180		
17	Acetone	1,2-Dichloroethane	--	5200	*	0.82	> 180	0.82	> 180		
18	Acetone	Epichlorohydrin	--	5200	*	0.14	> 180	0.14	> 180		
19	Acetone	Nitrobenzene	--	5200	*	0.02	> 180	0.02	> 180		
20	Acetone	Toluene	--	5200	*	0.01	> 180	0.01	> 180		
21	Acetone	Toluene	Methyl Ethyl Ketone	5200	*	0.01	> 180	0.01	> 180	0.01	> 180
22	Acetone	Toluene	Nitrobenzene	5200	*	0.02	> 180	0.02	> 180	0.02	> 180
23	Benzene	Dimethyl Sulfoxide	--	5200	*	0.01	> 180	0.01	> 180		
24	Benzene	Dimethyl Sulfoxide	1,2-Dichloroethane	5200	*	0.01	> 180	0.01	> 180	0.01	> 180
25	Chloroform	Dimethylformamide	--	5200	*	0.07	> 180	0.07	> 180		
26	Chloroform	Dimethyl Sulfoxide	--	5200	*	0.01	> 180	0.01	> 180		
27	Chloroform	Nitromethane	--	5200	*	0.55	> 180	0.55	> 180		
28	Methyl Ethyl Ketone	2-Nitropropane	Toluene	5200	*	0.82	> 180	0.82	> 180	0.82	> 180
29	Nitrobenzene	Toluene	--	5200	*	0.01	> 180	0.01	> 180		

* Reported MDL values did not indicate whether they were for specific mixture components or generic values for the mixture.

** Reported MDLs are generic mixture values. The breakthrough times report the time at which some component was detected but the specific component was not identified.

Source: U.S. Coast Guard Research and Development Center Testing Laboratory: Texas Research International

APPENDIX D

CHEMICAL MIXTURE PERMEATION TEST RESULTS
(ARTHUR D. LITTLE)

TABLE D-1. DATA REPORT FOR CARBON DISULFIDE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Carbon Disulfide	N/A	N/A
CAS Number:	75-15-0	N/A	N/A
Concentration:	Neat	N/A	N/A
Chemical Source:	Fisher		

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	23-24
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	7.7	N/A	N/A
Test System Sensitivity Factor:	2.3	N/A	N/A
Comments/Other Conditions:	none	N/A	N/A

TEST RESULTS

Date Tested:	See below
Number of Replicates:	3
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	41	N/A	N/A
Test Specimen #2	49	N/A	N/A
Test Specimen #3	49	N/A	N/A
Mean	46	N/A	N/A

TABLE D-1 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.63	N/A	N/A
Test Specimen #2	0.58	N/A	N/A
Test Specimen #3	0.54	N/A	N/A
Mean	0.58	N/A	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 7-31-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	4.1	1.58	N/A	N/A
2	12.2	1.58	N/A	N/A
3	44.7	7.51	N/A	N/A
4	101.5	54.12	N/A	N/A
5	125.9	88.09	N/A	N/A
6	166.5	152.47	N/A	N/A
7	190.8	189.21	N/A	N/A
8	223.3	237.00	N/A	N/A
9	247.7	271.37	N/A	N/A
10	288.3	341.28	N/A	N/A

Test Specimen 2:
Date Tested: 8-2-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	4.1	0.76	N/A	N/A
2	12.2	2.29	N/A	N/A
3	44.7	12.95	N/A	N/A
4	101.5	80.77	N/A	N/A
5	125.9	123.83	N/A	N/A
6	166.5	203.07	N/A	N/A
7	190.8	252.98	N/A	N/A
8	223.3	323.09	N/A	N/A
9	247.7	376.05	N/A	N/A
10	288.3	462.15	N/A	N/A

TABLE D-1 (Continued)

Test Specimen 3:
Date Tested: 8-3-89
Temperature (°C): 23

Data Point	Time (min)	Concentration (µg/L) Component 1	Component 2	Component 3
1	4.1	0.40	N/A	N/A
2	12.2	0.79	N/A	N/A
3	44.7	6.72	N/A	N/A
4	101.5	58.86	N/A	N/A
5	125.9	90.85	N/A	N/A
6	166.5	157.21	N/A	N/A
7	190.8	200.27	N/A	N/A
8	223.3	259.12	N/A	N/A
9	247.7	306.92	N/A	N/A
10	288.3	386.31	N/A	N/A

Other Observations: None

Source of Data: Arthur D. Little, Inc.
Acorn Park
Cambridge, MA 02140
(617) 864-5770

TABLE D-2. DATA REPORT FOR VINYL ACETATE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Vinyl Acetate	N/A	N/A
CAS Number:	108-05-04	N/A	N/A
Concentration:	Neat	N/A	N/A
Chemical Source:	Fisher	N/A	N/A

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	23-26
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	0.22	N/A	N/A
Test System Sensitivity Factor:	0.07	N/A	N/A
Comments/Other Conditions:	none	N/A	N/A

TEST RESULTS

Date Tested:	
Number of Replicates:	3
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	44	N/A	N/A
Test Specimen #2	22	N/A	N/A
Test Specimen #3	44	N/A	N/A
Mean	37	N/A	N/A

TABLE D-2 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.06	N/A	N/A
Test Specimen #2	0.06	N/A	N/A
Test Specimen #3	0.06	N/A	N/A
Mean	0.06	N/A	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 5-30-89
Temperature (°C): 26

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	1.9	0.14	N/A	N/A
2	50.0	0.37	N/A	N/A
3	101.8	1.70	N/A	N/A
4	149.9	5.02	N/A	N/A
5	201.6	11.13	N/A	N/A
6	253.4	19.34	N/A	N/A
7	301.5	28.40	N/A	N/A
8	353.3	38.81	N/A	N/A
9	401.4	48.43	N/A	N/A
10	453.2	58.23	N/A	N/A

Test Specimen 2:
Date Tested: 6-1-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	3.6	0.02	N/A	N/A
2	54.4	0.29	N/A	N/A
3	105.1	0.88	N/A	N/A
4	155.9	2.88	N/A	N/A
5	206.6	7.15	N/A	N/A
6	250.1	12.66	N/A	N/A
7	300.9	21.14	N/A	N/A
8	351.6	31.13	N/A	N/A
9	402.4	41.65	N/A	N/A
10	453.1	52.07	N/A	N/A

TABLE D-2 (Continued)

Test Specimen 3:
Date Tested: 6-5-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	3.6	0.08	N/A	N/A
2	54.5	0.27	N/A	N/A
3	105.1	0.96	N/A	N/A
4	155.9	2.88	N/A	N/A
5	206.6	6.98	N/A	N/A
6	250.1	12.31	N/A	N/A
7	300.9	20.50	N/A	N/A
8	351.6	30.07	N/A	N/A
9	402.4	40.00	N/A	N/A
10	453.1	50.06	N/A	N/A

Other Observations: None

Source of Data: Arthur D. Little, Inc.
Acorn Park
Cambridge, MA 02140
(617) 864-5770

TABLE D-3. DATA REPORT FOR ETHANOL PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Ethanol	N/A	N/A
CAS Number:	64-17-5	N/A	N/A
Concentration:	Neat	N/A	N/A
Chemical Source:	Fisher	N/A	N/A

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	23-24
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	3.0	N/A	N/A
Test System Sensitivity Factor:	0.9	N/A	N/A
Comments/Other Conditions:	none	N/A	N/A

TEST RESULTS

Date Tested:	See below
Number of Replicates:	2
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	303	N/A	N/A
Test Specimen #2	250	N/A	N/A
Test Specimen #3	NT	N/A	N/A
Mean	277	N/A	N/A

TABLE D-3 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.0038	N/A	N/A
Test Specimen #2	0.0033	N/A	N/A
Test Specimen #3	NT	N/A	N/A
Mean	0.0036	N/A	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 8-1-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	8.9	3.37	N/A	N/A
2	44.6	3.17	N/A	N/A
3	116.0	3.25	N/A	N/A
4	151.7	3.25	N/A	N/A
5	205.3	3.17	N/A	N/A
6	258.8	3.58	N/A	N/A
7	312.4	4.24	N/A	N/A
8	348.1	4.77	N/A	N/A
9	401.6	5.39	N/A	N/A
10	455.2	6.17	N/A	N/A

Test Specimen 2:
Date Tested: 8-2-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	8.9	-0.08	N/A	N/A
2	44.6	0.00	N/A	N/A
3	116.0	-0.13	N/A	N/A
4	151.7	0.13	N/A	N/A
5	205.3	0.55	N/A	N/A
6	258.8	0.93	N/A	N/A
7	312.4	1.40	N/A	N/A
8	348.1	1.95	N/A	N/A
9	401.6	2.37	N/A	N/A
10	455.2	3.18	N/A	N/A

TABLE D-3 (Continued)

Other Observations:	None
Source of Data:	Arthur D. Little, Inc. Acorn Park Cambridge, MA 02140 (617) 864-5770

TABLE D-4. DATA REPORT FOR CARBON DISULFIDE (90%) AND VINYL ACETATE (10%) MIXTURE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Carbon Disulfide	Vinyl Acetate	N/A
CAS Number:	75-15-0	108-05-4	N/A
Concentration:	90%	10%	N/A
Chemical Source:	Fisher	Fisher	N/A

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	23-24
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	4.2	0.5	N/A
Test System Sensitivity Factor:	1.2	0.2	N/A
Comments/Other Conditions:	none	none	N/A

TEST RESULTS

Date Tested:	See below
Number of Replicates:	3
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	30	107	N/A
Test Specimen #2	48	144	N/A
Test Specimen #3	521	122	N/A
Mean	43	124	N/A

TABLE D-4 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.50	0.021	N/A
Test Specimen #2	0.50	0.017	N/A
Test Specimen #3	0.55	0.018	N/A
Mean	0.51	0.019	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 6-28-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	2.71	0.12	N/A
2	61.1	18.23	0.19	N/A
3	90.7	52.35	0.41	N/A
4	120.3	97.34	0.74	N/A
5	149.9	148.14	1.23	N/A
6	179.5	200.49	1.90	N/A
7	212.8	260.99	3.01	N/A
8	242.4	314.12	4.14	N/A
9	272.0	367.25	5.48	N/A
10	301.6	418.05	7.00	N/A

Test Specimen 2:
Date Tested: 6-28-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	1.72	0.20	N/A
2	61.1	11.98	0.28	N/A
3	90.7	34.64	0.36	N/A
4	120.3	67.99	0.50	N/A
5	149.9	107.75	0.74	N/A
6	179.5	152.22	1.11	N/A
7	212.8	204.82	1.68	N/A
8	242.4	253.58	2.36	N/A
9	272.0	304.06	3.24	N/A
10	301.6	354.13	4.35	N/A

TABLE D-4 (Continued)

Test Specimen 3:
Date Tested: 6-30-89
Temperature (°C): 23

Data Point	Time (min)	Concentration (µg/L) Component 1	Component 2	Component 3
1	31.5	2.57	0.09	N/A
2	61.1	12.83	0.11	N/A
3	90.7	36.34	0.13	N/A
4	120.3	71.39	0.23	N/A
5	149.9	112.01	0.48	N/A
6	179.5	157.34	0.89	N/A
7	212.8	212.93	1.48	N/A
8	242.4	264.26	2.24	N/A
9	272.0	318.60	3.23	N/A
10	301.6	373.37	4.40	N/A

Other Observations: None

Source of Data: Arthur D. Little, Inc.
Acorn Park
Cambridge, MA 02140
(617) 864-5770

TABLE D-5. DATA REPORT FOR CARBON DISULFIDE (50%) AND VINYL ACETATE (50%) MIXTURE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Carbon Disulfide	Vinyl Acetate	N/A
CAS Number:	75-15-0	108-05-4	N/A
Concentration:	50%	50%	N/A
Chemical Source:	Fisher	Fisher	N/A

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	20-24
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	5.7	0.6	N/A
Test System Sensitivity Factor:	1.7	0.2	N/A
Comments/Other Conditions:	none	none	N/A

TEST RESULTS

Date Tested:	See below
Number of Replicates:	3
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	59	89	N/A
Test Specimen #2	59	78	N/A
Test Specimen #3	52	93	N/A
Mean	57	87	N/A

TABLE D-5 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.41	0.041	N/A
Test Specimen #2	0.40	0.035	N/A
Test Specimen #3	0.56	0.047	N/A
Mean	0.46	0.041	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 5-31-89
Temperature (°C): 20

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	-0.35	0.25	N/A
2	61.1	6.31	0.40	N/A
3	90.7	20.32	0.62	N/A
4	120.3	42.40	1.03	N/A
5	149.9	68.68	1.73	N/A
6	179.5	98.11	2.58	N/A
7	209.1	131.05	3.83	N/A
8	242.4	169.94	5.64	N/A
9	272.0	205.68	7.73	N/A
10	301.6	243.88	10.22	N/A

Test Specimen 2:
Date Tested: 6-9-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	0.00	0.21	N/A
2	61.1	9.19	0.37	N/A
3	90.7	27.57	0.65	N/A
4	120.3	52.20	1.05	N/A
5	149.9	80.87	1.64	N/A
6	179.5	113.22	2.51	N/A
7	209.1	144.83	3.67	N/A
8	242.4	186.01	5.50	N/A
9	272.0	225.71	7.57	N/A
10	301.6	266.88	10.04	N/A

TABLE D-5 (Continued)

Test Specimen 3:
Date Tested: 6-27-89
Temperature (°C): 24

Data Point	Time (min)	Concentration (µg/L) Component 1	Component 2	Component 3
1	31.5	1.94	0.51	N/A
2	61.1	12.02	0.65	N/A
3	90.7	34.13	0.89	N/A
4	120.3	67.09	1.47	N/A
5	149.9	107.81	2.49	N/A
6	179.5	154.34	4.01	N/A
7	209.1	206.31	6.34	N/A
8	242.4	268.36	9.73	N/A
9	272.0	324.59	13.57	N/A
10	301.6	383.15	18.00	N/A

Other Observations: None

Source of Data: Arthur D. Little, Inc.
Acorn Park
Cambridge, MA 02140
(617) 864-5770

TABLE D-6. DATA REPORT FOR CARBON DISULFIDE (10%) AND VINYL ACETATE (90%) MIXTURE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Carbon Disulfide	Vinyl Acetate	N/A
CAS Number:	75-15-0	108-05-4	N/A
Concentration:	10%	90%	N/A
Chemical Source:	Fisher	Fisher	N/A

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	23-26
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	14.7	0.5	N/A
Test System Sensitivity Factor:	4.4	0.2	N/A
Comments/Other Conditions:	none	none	N/A

TEST RESULTS

Date Tested:	See below
Number of Replicates:	3
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	89	89	N/A
Test Specimen #2	52	26	N/A
Test Specimen #3	85	67	N/A
Mean	75	61	N/A

TABLE D-6 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.36	0.066	N/A
Test Specimen #2	0.28	0.065	N/A
Test Specimen #3	0.25	0.046	N/A
Mean	0.30	0.059	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 6-21-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	1.27	0.06	N/A
2	61.1	6.78	0.10	N/A
3	90.7	15.26	0.32	N/A
4	120.3	28.42	0.87	N/A
5	149.9	45.42	1.91	N/A
6	183.1	65.87	3.77	N/A
7	212.7	86.79	5.14	N/A
8	242.3	109.44	9.13	N/A
9	271.9	131.28	12.57	N/A
10	301.5	151.04	16.37	N/A

Test Specimen 2:
Date Tested: 6-21-89
Temperature (°C): 26

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	3.84	0.38	N/A
2	61.1	14.45	0.79	N/A
3	90.7	32.71	1.73	N/A
4	120.3	55.28	3.52	N/A
5	149.9	81.74	6.49	N/A
6	183.1	112.55	11.01	N/A
7	212.7	141.71	16.11	N/A
8	242.3	170.08	21.89	N/A
9	271.9	198.91	28.18	N/A
10	301.5	227.33	34.67	N/A

TABLE D-6 (Continued)

Test Specimen 3:
Date Tested: 6-22-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	3.83	0.33	N/A
2	61.1	8.51	0.61	N/A
3	90.7	22.51	1.16	N/A
4	120.3	41.21	2.19	N/A
5	149.9	62.07	3.86	N/A
6	183.1	88.94	6.69	N/A
7	212.7	114.60	10.15	N/A
8	242.3	139.45	14.19	N/A
9	271.9	165.18	18.78	N/A
10	301.5	189.67	23.53	N/A

Other Observations: None

Source of Data: Arthur D. Little, Inc.
Acorn Park
Cambridge, MA 02140
(617) 864-5770

TABLE D-7. DATA REPORT FOR CARBON DISULFIDE (50%) AND ETHANOL (50%) MIXTURE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Carbon Disulfide	Ethanol	N/A
CAS Number:	75-15-0	64-17-5	N/A
Concentration:	50%	50%	N/A
Chemical Source:	Fisher	Fisher	N/A

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C)	26
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	7.3	5.0	N/A
Test System Sensitivity Factor:	2.1	1.5	N/A
Comments/Other Conditions:	none	none	N/A

TEST RESULTS

Date Tested:	See below
Number of Replicates:	2
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	37	426	N/A
Test Specimen #2	37	272	N/A
Test Specimen #3	NT	NT	N/A
Mean	37	349	N/A

TABLE D-7 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.74	No SSPR	N/A
Test Specimen #2	0.74	No SSPR	N/A
Test Specimen #3	NT	NT	N/A
Mean	0.74	No SSPR	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested:
Temperature (°C):

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	5.98	0.74	N/A
2	61.1	32.06	0.80	N/A
3	90.7	77.79	0.87	N/A
4	120.3	136.34	1.02	N/A
5	149.9	203.87	1.42	N/A
6	179.4	276.10	1.86	N/A
7	209.0	350.90	2.51	N/A
8	242.3	437.66	3.24	N/A
9	271.9	516.73	4.02	N/A
10	301.5	593.23	4.77	N/A

Test Specimen 2:
Date Tested: 7-31-89
Temperature (°C): 26

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	9.3	1.21	-0.17	N/A
2	31.5	3.64	-0.31	N/A
3	46.3	10.11	-0.54	N/A
4	57.4	19.42	-0.65	N/A
5	74.4	43.28	-0.66	N/A
6	125.0	123.37	-0.76	N/A
7	175.6	230.97	-0.31	N/A
8	226.2	347.06	0.05	N/A
9	276.8	472.86	1.25	N/A
10	327.4	598.26	2.27	N/A

TABLE D-7 (Continued)

Other Observations:	None
Source of Data:	Arthur D. Little, Inc. Acorn Park Cambridge, MA 02140 (617) 864-5770

TABLE D-8. DATA REPORT FOR VINYL ACETATE (50%) AND ETHANOL (50%) MIXTURE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Vinyl Acetate	Ethanol	N/A
CAS Number:	108-05-4	64-17-5	N/A
Concentration:	50%	50%	N/A
Chemical Source:	Fisher	Fisher	N/A

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	23
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	0.3	ND	N/A
Test System Sensitivity Factor:	0.1	--	N/A
Comments/Other Conditions:	none	none	N/A

TEST RESULTS

Date Tested:	See below
Number of Replicates:	2
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	137	ND	N/A
Test Specimen #2	4	ND	N/A
Test Specimen #3	NT	NT	N/A
Mean	71	ND	N/A

TABLE D-8 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.024	No SSPR	N/A
Test Specimen #2	0.027	No SSPR	N/A
Test Specimen #3	NT	NT	N/A
Mean	0.026	No SSPR	N/A

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 7-6-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	-0.13	-0.15	N/A
2	61.1	-0.16	-0.32	N/A
3	90.7	-0.13	-0.50	N/A
4	120.3	0.11	-0.41	N/A
5	149.9	0.48	-0.48	N/A
6	179.4	1.07	-0.55	N/A
7	212.7	2.00	-0.51	N/A
8	242.3	3.23	-0.36	N/A
9	271.9	4.65	-0.33	N/A
10	301.5	6.44	-0.36	N/A

Test Specimen 2:
Date Tested: 7-6-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	1.80	-0.12	N/A
2	61.1	2.80	-0.22	N/A
3	90.7	3.66	-0.38	N/A
4	120.3	4.57	-0.28	N/A
5	149.9	5.69	-0.40	N/A
6	179.4	7.11	-0.28	N/A
7	212.7	9.23	-0.10	N/A
8	242.3	11.48	-0.00	N/A
9	271.9	14.17	0.24	N/A
10	301.5	17.12	0.43	N/A

TABLE D-8 (Continued)

Other Observations:	None
Source of Data:	Arthur D. Little, Inc. Acorn Park Cambridge, MA 02140 (617) 864-5770

TABLE D-9. DATA REPORT FOR CARBON DISULFIDE (45%), VINYL ACETATE (45%), AND ETHANOL (10%) MIXTURE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Carbon Disulfide	Vinyl Acetate	Ethanol
CAS Number:	75-15-0	108-05-4	64-17-5
Concentration:	45%	45%	10%
Chemical Source:	Fisher	Fisher	Fisher

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	24
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	7.0	0.3	2.5
Test System Sensitivity Factor:	2.1	0.1	0.7
Comments/Other Conditions:	none	none	none

TEST RESULTS

Date Tested:	See below
Number of Replicates:	2
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	41	67	352
Test Specimen #2	41	74	433
Test Specimen #3	NT	NT	NT
Mean	41	71	393

TABLE D-9 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.66	0.052	No SSPR
Test Specimen #2	0.64	0.050	No SSPR
Test Specimen #3	NT	NT	NT
Mean	0.65	0.051	No SSPR

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 7-12-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	4.32	0.09	0.20
2	61.1	24.62	0.19	0.25
3	90.7	63.50	0.66	0.27
4	120.3	114.48	1.59	0.15
5	149.9	174.53	3.23	0.47
6	179.4	239.76	5.68	0.38
7	212.7	317.52	9.36	0.60
8	242.3	388.37	13.38	0.72
9	271.9	457.92	17.86	1.07
10	301.5	527.04	22.93	1.41

Test Specimen 2:
Date Tested: 7-13-89
Temperature (°C): 24

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	2.16	-0.01	-0.13
2	61.1	23.76	0.13	-0.09
3	90.7	62.64	0.58	-0.12
4	120.3	111.46	1.53	-0.15
5	149.9	169.34	3.06	-0.12
6	179.4	230.26	5.27	0.06
7	212.7	301.10	8.44	0.15
8	242.3	366.34	11.95	0.19
9	271.9	432.43	16.00	0.58
10	301.5	505.87	21.00	0.88

TABLE D-9 (Continued)

Other Observations:	None
Source of Data:	Arthur D. Little, Inc. Acorn Park Cambridge, MA 02140 (617) 864-5770

TABLE D-10. DATA REPORT FOR CARBON DISULFIDE (25%), VINYL ACETATE (25%), AND ETHANOL (50%) MIXTURE PERMEATION TESTS

DESCRIPTION OF PRODUCT EVALUATED

Condition Before Test:	Flat sheet material
Manufacturer:	Chemical Fabrics Corporation
Product Identification:	Challenge 5200
Nominal Thickness (mm):	0.27
Material Type:	Teflon
Description:	Teflon-Glass Fiber-Teflon

CHALLENGE CHEMICAL

	Component 1	Component 2	Component 3
Chemical Name:	Carbon Disulfide	Vinyl Acetate	Ethanol
CAS Number:	75-15-0	108-05-4	64-17-5
Concentration:	25%	25%	50%
Chemical Source:	Fisher	Fisher	Fisher

TEST METHOD

Standard Test Method Used:	ASTM F739
Deviations From Standard Test Method:	None
Testing Laboratory:	Arthur D. Little, Inc., Cambridge, MA 02140
Analytical Method:	IR
Temperature (°C):	23
Specimen Area Exposed (cm^2):	20.27
Collection System:	Closed-Loop (Recirculating)
Collection Medium:	Air
Collection Medium Volume (L):	6
Collection Medium Flowrate (L/min):	10

	Component 1	Component 2	Component 3
Ave. Breakthrough Concentration (µg/L):	6.8	0.3	ND
Test System Sensitivity Factor:	2	0.1	--
Comments/Other Conditions:	none	none	none

TEST RESULTS

Date Tested:	See below
Number of Replicates:	2
Location Sampled From:	Random sample from sheet stock

	Component 1	Component 2	Component 3
Breakthrough Time (min:)			
Test Specimen #1	44	81	444
Test Specimen #2	52	111	ND
Test Specimen #3	NT	NT	NT
Mean	48	96	>444

TABLE D-10 (Continued)

Steady-State Perm. Rate ($\mu g/cm^2/min$):			
Test Specimen #1	0.50	0.034	No SSPR
Test Specimen #2	0.54	0.036	No SSPR
Test Specimen #3	NT	NT	NT
Mean	0.51	0.035	No SSPR

SELECTED DATA POINTS

Test Specimen 1:
Date Tested: 6-28-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	2.61	0.11	0.15
2	61.1	15.21	0.17	0.21
3	90.7	43.03	0.40	0.07
4	120.3	79.97	0.87	0.34
5	149.9	122.56	1.62	0.40
6	179.4	169.49	2.78	0.46
7	212.7	225.99	4.56	0.71
8	242.3	278.14	6.66	0.94
9	301.5	378.97	11.65	1.53
10	331.1	428.95	14.62	1.99

Test Specimen 2:
Date Tested: 6-28-89
Temperature (°C): 23

		Concentration (µg/L)		
Data Point	Time (min)	Component 1	Component 2	Component 3
1	31.5	1.74	-0.08	-0.15
2	61.1	12.60	-0.12	-0.16
3	90.7	39.11	0.07	-0.20
4	120.3	73.45	0.45	-0.08
5	149.9	112.13	1.08	-0.17
6	179.4	156.02	2.05	-0.07
7	212.7	209.91	3.61	0.17
8	242.3	259.89	5.44	0.32
9	301.5	365.50	10.26	0.98
10	331.1	421.13	13.26	1.31

TABLE D-10 (Continued)

Other Observations:	None
Source of Data:	Arthur D. Little, Inc. Acorn Park Cambridge, MA 02140 (617) 864-5770

APPENDIX E

FICK'S LAW DATA ANALYSIS PROCEDURES

The available permeation-time curves were analyzed to assess whether the behavior could be accurately described by a solution-diffusion mechanism using Fick's laws of diffusion. As reported in Section 4, mathematical relationships based on Fick's law describe the permeation rate, J, and the cumulative amount permeated, M, at any time following initiation of chemical contact. These relationships require two fundamental parameters: the diffusion coefficient, D, and the solubility, S, of the permeant in the material of interest:

$$J=(DS/l)[1+2\sum_{n=1}^{\infty}(-1)^n\exp(-\pi^2n^2\psi)] \qquad \text{Eq. (E-1)}$$

and

$$M = (Sl)[\psi-1/6-2\sum_{n=1}^{\infty}[(-1)^n/(\pi n)^2]\exp(-(n\pi)^2\psi)] \qquad \text{Eq. (E-2)}$$

where J = permeation rate, $\mu g/cm^2$-min
M = cumulative amount permeated, $\mu g/cm^2$
ψ = Dt/l^2, dimensionless
D = diffusion coefficient, cm^2/min
S = equilibrium solubility, $\mu g/cm^3$
l = membrane thickness, cm
t = time, min

These equations can be used to solve for values of D and S given a set of J versus t or M versus t data. For the permeation test results analyzed in this effort, the permeation-time curves provide sets of J versus t data that can also be converted to M versus t data by analysis of the areas under the curves at various times. Two approaches to extract D and S values were pursued depending on the type of curve available. For permeation curves in which steady-state was reached, values for D and S were solved for directly using Eq. (E-2). For permeation-time curves in which permeation rates were still increasing with time, values for D and S were determined using Eq. (E-1) and an iterative curve-fitting technique.

STEADY-STATE PERMEATION CURVE ANALYSIS

For permeation-time curves that reached steady-state, values for D and S were calculated by applying Eq. (E-2) at long times (i.e., when steady-state is reached). At steady-state, Eq (E-2) predicts that M increases linearly with time with a slope equal to the steady-state permeation rate that is defined by D, S, and *l*:

$$M = (Slope)(t) + Intercept \qquad \text{Eq. (E-3)}$$

where:

$$Slope = DS/l \qquad \text{Eq. (E-4)}$$

The intercept of Eq. (E-3) with the y-axis (or the value at which t equals 0) is defined from Eq. (E-2) as:

$$Intercept = (-Sl)/6 \qquad \text{Eq. (E-5)}$$

Thus, by analyzing the M versus t data at steady-state, one can calculate the slope and intercept of Eq. (E-3) and directly calculate a value for S given the barrier film thickness, *l*. Using this value for S, one can calculate a value for D using Eq. (E-4). The value of D can be separately confirmed by calculating the lag time, t_L, or the time at which M calculated by Eq (E-3) equals 0:

$$t_L = l^2/6D \qquad \text{Eq. (E-6)}$$

Thus,

$$D = l^2/6t_L \qquad \text{Eq. (E-7)}$$

Use of this direct approach is only possible when the permeation-time data have reached steady state.

TRANSIENT CURVE ANALYSIS

For permeation-time curves that have not reached steady-state, values for D and S must be calculated from the data in the transient portion of the curve. In this region, however, Eq. (E-1) and (E-2) can not be simplified to solve for D and S directly. In this case, though, we can analyze subsequent sets of (J,t) data points so as to eliminate S from the equation and solve for D through an iterative curve fitting technique. Once D is determined, a value for S can be calculated that also best fits the data.

In this analysis technique, we use the ratio of two permeation rates (J_1/J_2) by dividing Eq. (E-1) by itself at two separate time intervals, t_1 and t_2:

$$\frac{J_2}{J_1} = \frac{(DS/l)[1+2\sum_{n=1}^{\infty}(-1)^n\exp(-\pi^2n^2\psi_2)]}{(DS/l)[1+2\sum_{n=1}^{\infty}(-1)^n\exp(-\pi^2n^2\psi_1)]} \qquad \text{Eq. (E-8)}$$

Thus, the leading term in each equation drops out and S is eliminated:

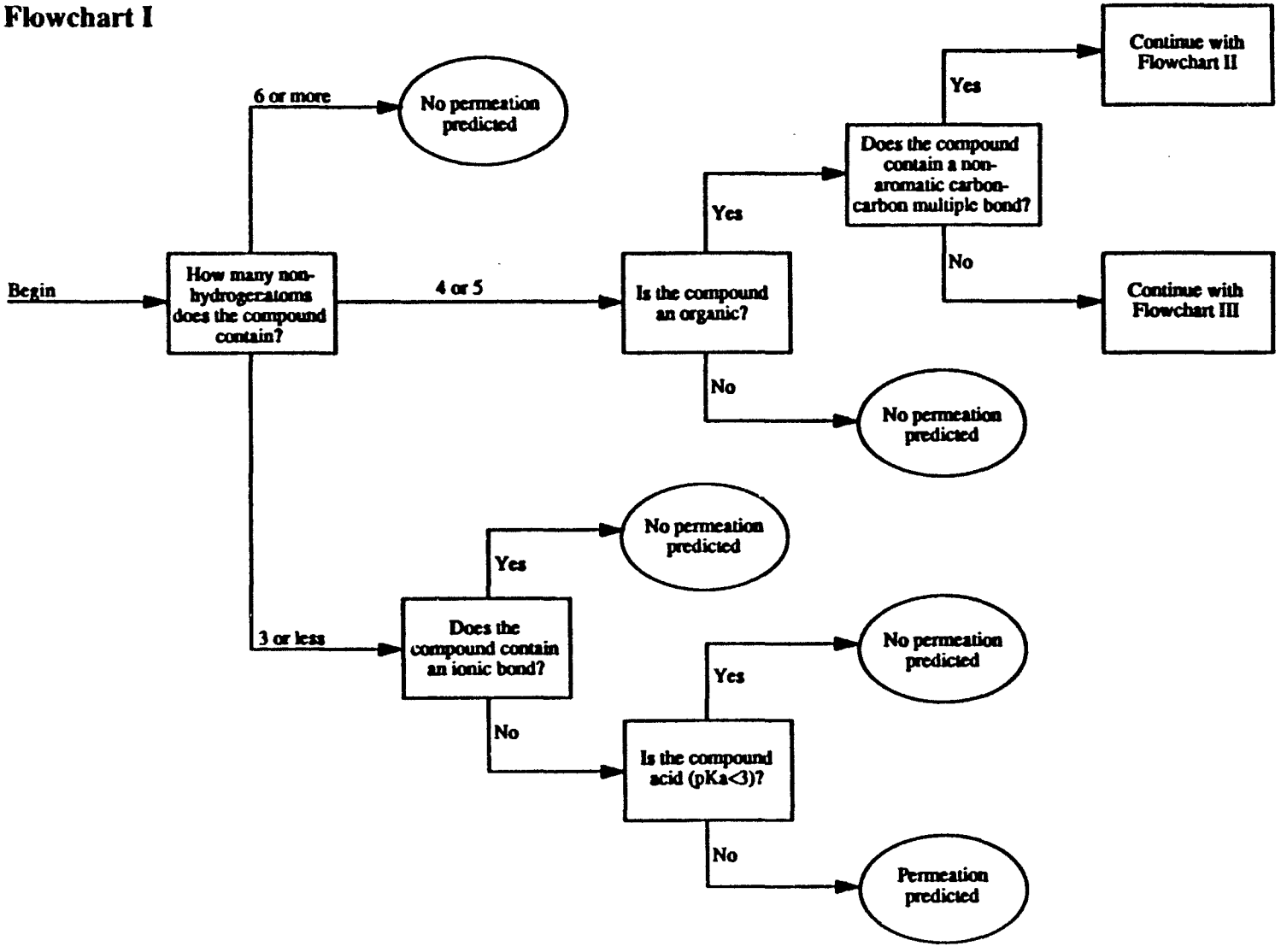
$$\frac{J_2}{J_1} = \frac{[1+2\sum_{n=1}^{\infty}(-1)^n\exp(-\pi^2n^2\psi_2)]}{[1+2\sum_{n=1}^{\infty}(-1)^n\exp(-\pi^2n^2\psi_1)]} \qquad \text{Eq. (E-9)}$$

Since J_1, J_2, t_1, and t_2 are known, a value for D can be calculated. An average or best fit value of D is determined by analyzing various pairs of (J,t) data points from the transition region of the permeation-time curve. Then, using Eq. (E-1) a value for S can be fit using the values for D and *l*.

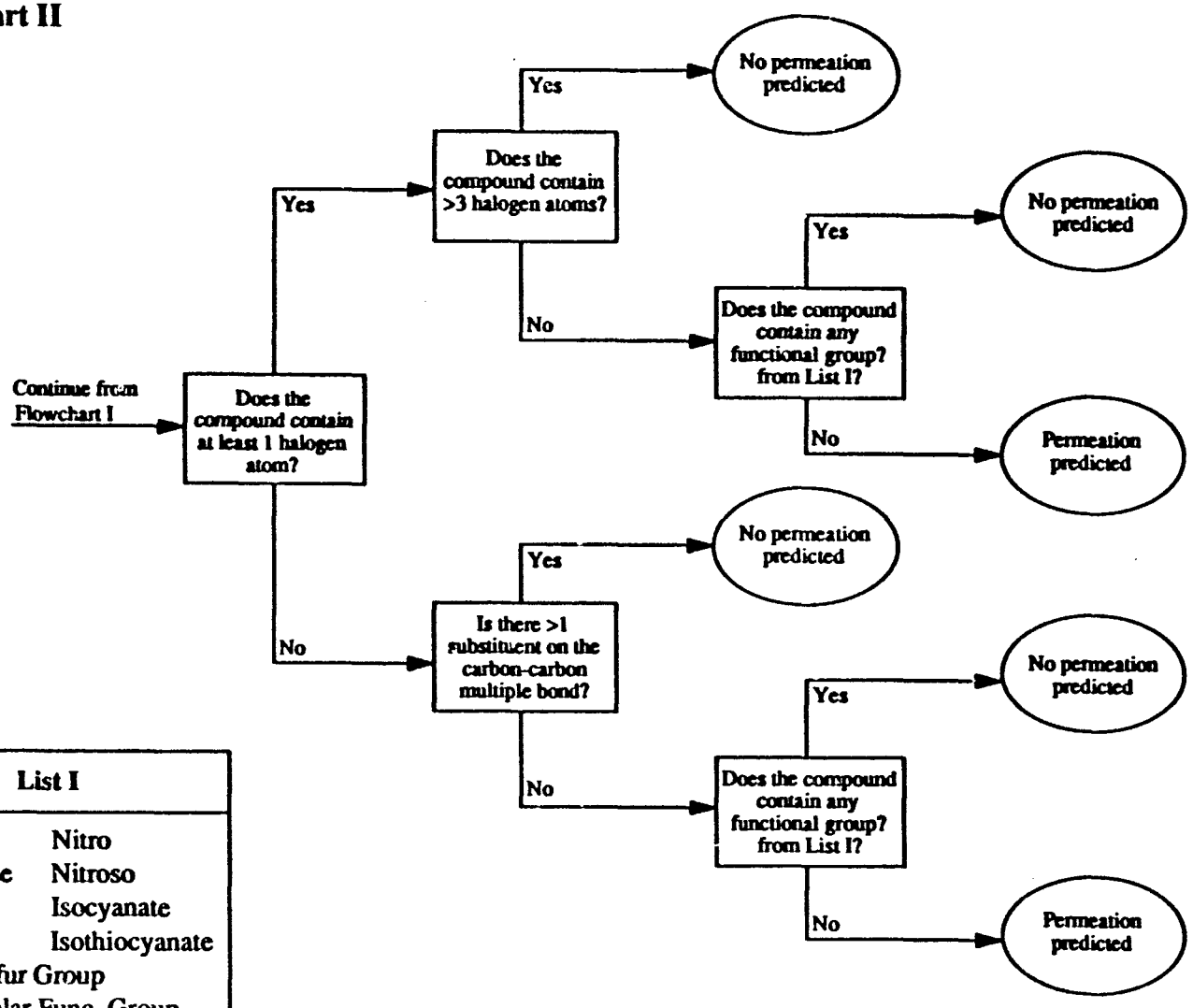
APPENDIX F

EMPIRICAL MODEL DECISION TREE

Flowchart I


Begin
How many non-hydrogen atoms does the compound contain?
6 or more
No permeation predicted
4 or 5
Is the compound an organic?
Yes
Does the compound contain a non-aromatic carbon-carbon multiple bond?
Yes
Continue with Flowchart II
No
Continue with Flowchart III
No
No permeation predicted
3 or less
Does the compound contain an ionic bond?
Yes
No permeation predicted
No
Is the compound acid (pKa<3)?
Yes
No permeation predicted
No
Permeation predicted

Flowchart II



List I	
Alcohol	Nitro
Aldehyde	Nitroso
Amine	Isocyanate
Ketone	Isothiocyanate
Any Sulfur Group	
Other Polar Func. Group	

Flowchart III